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Non-equilibrium quantum systems

(Potentially useful lecture-note material)

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Preface

Here is a collection of notes which contain material relevant to the Course on "Non-equilibrium quantum systems" held within the Spring College on "Physics of Complex Systems". The material has no pretense of being coherently organized in any way. Being a "collage" of different lecture notes, please be aware that even the LaTex is not perfectly consistent: there might be undefined references, or multiply defined labels. Sorry, this is not a book.

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1. Quantum Ising chains

The present chapter presents, in a rather dry way, the technical machinery to deal with Quantum Ising spin chains. We start with one of the basic techniques that allows an exact treatment of many one-dimensional models: the Jordan-Wigner transformation.

1.1. Jordan-Wigner transformation

We first transform the Pauli spin-1/2 operators $\hat{\sigma}_j^\alpha$ (with $\alpha = x, y, z$, and j a generic site index) into *hard-core bosons* $\hat{b}_j^\dagger$, by identifying, at each site, $|0\rangle \leftrightarrow |\downarrow\rangle$ and $|1\rangle = \hat{b}^\dagger|0\rangle \leftrightarrow |\uparrow\rangle$. Defining [1] $\hat{\sigma}^\pm = (\hat{\sigma}^x \pm i\hat{\sigma}^y)/2$ which act as $\hat{\sigma}^+|\downarrow\rangle = |\uparrow\rangle$, $\hat{\sigma}^-|\uparrow\rangle = |\downarrow\rangle$, we must evidently have:

$$\left\{ \begin{array}{lcl} \hat{\sigma}_j^+ &=& \hat{b}_j^\dagger \\ \hat{\sigma}_j^- &=& \hat{b}_j \\ \hat{\sigma}_j^z &=& 2\hat{b}_j^\dagger \hat{b}_j - 1 \end{array} \right. \quad \Longrightarrow \quad \left\{ \begin{array}{lcl} \hat{\sigma}_j^x &=& \hat{b}_j^\dagger + \hat{b}_j \\ \hat{\sigma}_j^y &=& -i(\hat{b}_j^\dagger - \hat{b}_j) \\ \hat{\sigma}_j^z &=& 2\hat{b}_j^\dagger \hat{b}_j - 1 \end{array} \right. . \tag{1.1}$$

These operators $\hat{b}_j^\dagger$ commute at different sites — as the original $\hat{\sigma}_j^\alpha$ do — but are not ordinary bosonic operators, [2] because they must verify the hard-core constraint $(\hat{b}_j^\dagger)^2|0\rangle = 0$, i.e., *at most one boson* is allowed on each site. The hard-core constraint seems to be ideally representable in terms of *spinless fermions* $\hat{c}_j^\dagger$, where the absence of double occupancy is automatically enforced by the *Pauli exclusion principle*, and the anticommutation on the same site comes for free.

Unfortunately, whereas the mapping of $\hat{\sigma}_j^\alpha$ into hard-core bosons $\hat{b}_j^\dagger$ is true in any spatial dimension (albeit of rather limited usefulness), the writing of the $\hat{b}_j^\dagger$ in terms of spinless fermions $\hat{c}_j^\dagger$ is really possible/useful only in *one-dimension*, where a natural ordering of sites is possible, [3] $j = 1, 2, \cdots, L$. In other words, because fermion operators on different sites must anticommute, the exact handling of the resulting minus signs — which are absent in the original spin problem — is possible only in one-dimension (1D), through the Jordan-Wigner transformation. The Jordan-Wigner transformation of hard-core bosons into fermions reads:

$$\hat{b}_j = K_j \hat{c}_j = \mathrm{e}^{i\pi \sum_{j'=1}^{j-1} \hat{n}_{j'}} \hat{c}_j = \left[\prod_{j'=1}^{j-1} (1 - 2\hat{n}_{j'}) \right] \hat{c}_j \ , \tag{1.2}$$

where the *non-local* string operator K_j is simply a *sign*, $K_j = \pm 1$, counting the parity of the number of fermions which sit *before* site j (i.e., between site 1 and site $j-1$), which

[1] Notice the factor 1/2, which is not entirely standard. With this definition $\hat{\sigma}^\pm = s^\pm/\hbar$.

[2] In particular, on the same site $\{\hat{\sigma}_j^-, \hat{\sigma}_j^+\} = 1$ and this implies that $\{\hat{b}_j, \hat{b}_j^\dagger\} = 1$, while ordinary bosons would have the commutator $[\hat{b}_j, \hat{b}_j^\dagger] = 1$.

[3] We start by assuming a chain of finite size L, and take the thermodynamic limit $L \to \infty$ only at the end.

multiplies the operator $\hat{c}_j$. (Notice that $K_j = K_j^\dagger = K_j^{-1}$, and $K_j^2 = 1$.) Here $\hat{n}_j = \hat{c}_j^\dagger \hat{c}_j$ is the fermion number operator, but one can show that the phase-factor K_j cancels out in it, i.e., $\hat{n}_j = \hat{c}_j^\dagger \hat{c}_j = \hat{b}_j^\dagger \hat{b}_j$. Let us prove that everything works fine. More precisely, we will now show that if the $\hat{c}_j$ are taken to be standard fermionic operators, with canonical *anticommutation* relations $\{\hat{c}_j, \hat{c}_{j'}^\dagger\} = \delta_{j,j'}$ and $\{\hat{c}_j, \hat{c}_{j'}\} = \{\hat{c}_j^\dagger, \hat{c}_{j'}^\dagger\} = 0$, then the following two properties of the $\hat{b}_j$ follow:

$$\begin{aligned} \textbf{P1} \quad &: \quad \left\{\hat{b}_j, \hat{b}_j^\dagger\right\} = 1 \\ \textbf{P2} \quad &: \quad \left(\begin{array}{ll} \left[\hat{b}_{j_1}, \hat{b}_{j_2}^\dagger\right] = 0 & \\ \left[\hat{b}_{j_1}, \hat{b}_{j_2}\right] = 0 & \text{if } j_1 \neq j_2 \ , \\ \left[\hat{b}_{j_1}^\dagger, \hat{b}_{j_2}^\dagger\right] = 0 & \end{array} \right. \end{aligned} \tag{1.3}$$

i.e., in other words, the $\hat{b}_j$ are *hard-core bosons*. Property **P1** is straightforward because the string factor K_j cancels completely:

$$\hat{b}_j^\dagger \hat{b}_j = \hat{c}_j^\dagger K_j^\dagger K_j \hat{c}_j = \hat{c}_j^\dagger \hat{c}_j \ ,$$

and, similarly, $\hat{b}_j \hat{b}_j^\dagger = \hat{c}_j \hat{c}_j^\dagger$. In essence, on each site the $\hat{b}_j$ inherit the anticommutation property **P1** from the fermions $\hat{c}_j$. To prove **P2**, let us consider $\left[\hat{b}_{j_1}, \hat{b}_{j_2}^\dagger\right]$, assuming $j_2 > j_1$. Using Eq. (1.2), it is simple to show that

$$\hat{b}_{j_1} \hat{b}_{j_2}^\dagger = \hat{c}_{j_1} \mathrm{e}^{-i\pi \sum_{j=j_1}^{j_2-1} \hat{n}_j} \hat{c}_{j_2}^\dagger \ . \tag{1.4}$$

Similarly, you can show that

$$\begin{aligned} \hat{b}_{j_2}^\dagger \hat{b}_{j_1} &= \hat{c}_{j_2}^\dagger \mathrm{e}^{-i\pi \sum_{j=j_1}^{j_2-1} \hat{n}_j} \hat{c}_{j_1} = \mathrm{e}^{-i\pi \sum_{j=j_1}^{j_2-1} \hat{n}_j} \hat{c}_{j_2}^\dagger \hat{c}_{j_1} \\ &= -\mathrm{e}^{-i\pi \sum_{j=j_1}^{j_2-1} \hat{n}_j} \hat{c}_{j_1} \hat{c}_{j_2}^\dagger = +\hat{c}_{j_1} \mathrm{e}^{-i\pi \sum_{j=j_1}^{j_2-1} \hat{n}_j} \hat{c}_{j_2}^\dagger \ , \end{aligned} \tag{1.5}$$

where the change of sign in the second line is due to the fermionic anticommutation, while the crucial final change of sign is due to the fact that $\hat{n}_{j_1} = 0$ at the beginning of the second line, while $\hat{n}_{j_1} = 1$ in the final expression, because of the neighboring action of $\hat{c}_{j_1}$. Comparing Eq. (1.4) with Eq. (1.5), you immediately deduce that $\left[\hat{b}_{j_1}, \hat{b}_{j_2}^\dagger\right] = 0$. In a similar way all the other commutations relationship of **P2** are shown.

Here is a summary of a few useful expressions where the string operator K_j disappears exactly:

$$\begin{aligned} \hat{b}_j^\dagger \hat{b}_j &= \hat{c}_j^\dagger \hat{c}_j \ , \\ \hat{b}_j^\dagger \hat{b}_{j+1}^\dagger &= \hat{c}_j^\dagger (1 - 2\hat{n}_j) \hat{c}_{j+1}^\dagger = \hat{c}_j^\dagger \hat{c}_{j+1}^\dagger \ , \\ \hat{b}_j^\dagger \hat{b}_{j+1} &= \hat{c}_j^\dagger (1 - 2\hat{n}_j) \hat{c}_{j+1} = \hat{c}_j^\dagger \hat{c}_{j+1} \\ \hat{b}_j \hat{b}_{j+1} &= \hat{c}_j (1 - 2\hat{n}_j) \hat{c}_{j+1} = \hat{c}_j (1 - 2(1 - \hat{c}_j \hat{c}_j^\dagger)) \hat{c}_{j+1} = -\hat{c}_j \hat{c}_{j+1} \\ \hat{b}_j \hat{b}_{j+1}^\dagger &= \hat{c}_j (1 - 2\hat{n}_j) \hat{c}_{j+1}^\dagger = \hat{c}_j (1 - 2(1 - \hat{c}_j \hat{c}_j^\dagger)) \hat{c}_{j+1}^\dagger = -\hat{c}_j \hat{c}_{j+1}^\dagger \end{aligned} \tag{1.6}$$

Notice the minus signs on the right hand side, which should not be forgotten. Notice also that we have used

$$\prod_{j'=1}^{j-1} (1 - 2\hat{n}_{j'}) \prod_{j'=1}^{j} (1 - 2\hat{n}_{j'}) = 1 - 2\hat{n}_j \ . \tag{1.7}$$

since $(1-2\hat{n}_{j'})(1-2\hat{n}_{j'})=1$, and terms with different site-index commute.

Armed with these expression, it is simple to show which spin operators transform in a simple way into local fermionic operators. Here is a short summary:

$$\begin{aligned}
\hat{\sigma}^z_j &= 2\hat{n}_j - 1 \\
\hat{\sigma}^x_j\hat{\sigma}^x_{j+1} &= \left(\hat{b}^\dagger_j\hat{b}^\dagger_{j+1} + \hat{b}^\dagger_j\hat{b}_{j+1} + H.c.\right) = \left(\hat{c}^\dagger_j\hat{c}^\dagger_{j+1} + \hat{c}^\dagger_j\hat{c}_{j+1} + H.c.\right) \\
\hat{\sigma}^y_j\hat{\sigma}^y_{j+1} &= -\left(\hat{b}^\dagger_j\hat{b}^\dagger_{j+1} - \hat{b}^\dagger_j\hat{b}_{j+1} + H.c.\right) = -\left(\hat{c}^\dagger_j\hat{c}^\dagger_{j+1} - \hat{c}^\dagger_j\hat{c}_{j+1} + H.c.\right) \ . \qquad (1.8)
\end{aligned}$$

One important point to note concerns boundary conditions. One often assumes periodic boundary conditions (PBC) for the spin operators, which in turns immediately implies the same PBC conditions for the hard-core bosons, that is, e.g., $\hat{b}^\dagger_L\hat{b}_{L+1} \equiv \hat{b}^\dagger_L\hat{b}_1$. But now look what happens when we rewrite a term of this form using spinless fermions:

$$\hat{b}^\dagger_L\hat{b}_1 = \mathrm{e}^{i\pi\sum_{j'=1}^{L-1}\hat{n}_{j'}}\hat{c}^\dagger_L\hat{c}_1 = -\mathrm{e}^{i\pi\sum_{j'=1}^{L}\hat{n}_{j'}}\hat{c}^\dagger_L\hat{c}_1 = -(-1)^{N_F}\hat{c}^\dagger_L\hat{c}_1 \ , \qquad (1.9)$$

where the second equality follows because, to the left of $\hat{c}^\dagger_L$ we certainly have $\hat{n}_L = 1$, and therefore the factor $-\mathrm{e}^{i\pi\hat{n}_L} \equiv 1$. Similarly, you can verify that:

$$\hat{b}^\dagger_L\hat{b}^\dagger_1 = \mathrm{e}^{i\pi\sum_{j'=1}^{L-1}\hat{n}_{j'}}\hat{c}^\dagger_L\hat{c}^\dagger_1 = -\mathrm{e}^{i\pi\sum_{j'=1}^{L}\hat{n}_{j'}}\hat{c}^\dagger_L\hat{c}^\dagger_1 = -(-1)^{N_F}\hat{c}^\dagger_L\hat{c}^\dagger_1 \ . \qquad (1.10)$$

This shows that boundary conditions are affected by the *fermion parity* $(-1)^{N_F}$, and PBC become antiperiodic boundary condition (ABC) when N_F is *even*. No problem whatsoever is present, instead, when the boundary conditions are *open*, OBC, because there is no link, in the Hamiltonian, between operators at site L and operators at site $L+1 \equiv 1$.

1.2. Transverse field Ising model: fermionic formulation

Let us now concentrate on a class of one-dimensional models where the resulting fermionic Hamiltonian can be exactly diagonalized, because it is quadratic: such a class includes the XY model, and the Ising model in a transverse field. The model we want to study is the one-dimensional random Ising chain, possibly with XY anisotropy, in presence of a transverse field. After a rotation in spin-space, we can always rewrite the Hamiltonian as follows:

$$\hat{H} = -\sum_j \left(J^x_j\hat{\sigma}^x_j\hat{\sigma}^x_{j+1} + J^y_j\hat{\sigma}^y_j\hat{\sigma}^y_{j+1}\right) + \sum_j h_j\hat{\sigma}^z_j \ , \qquad (1.11)$$

where $\hat{\sigma}^\alpha_j$ are Pauli matrices. The couplings $J^{x,y}_j$ and the transverse fields h_j can be chosen, for instance, as independent random variables with uniform distribution. For a system of finite size L with open boundary condition (OBC), the first sum runs over $j = 1, \cdots, L-1$, the second over $j = 1, \cdots, L$. If periodic boundary conditions (PBC) are chosen, both sums run over $j = 1, \cdots, L$ and one assumes that $\hat{\sigma}^\alpha_{L+1} \equiv \hat{\sigma}^\alpha_1$. For $J^y_j = 0$ we have the Ising model in a transverse field, for $J^y_j = J^x_j$ the istropic XY model.

In terms of bosons, the Hamiltonian becomes:

$$\hat{H} = -\sum_j \left[J^+_j(\hat{b}^\dagger_j\hat{b}_{j+1} + H.c.) \ + \ J^-_j(\hat{b}^\dagger_j\hat{b}^\dagger_{j+1} + H.c.)\right] + \sum_j h_j(2\hat{n}_j - 1) \ ,$$

where the shorthand notation for the couplings $J_i^{\pm} = J_j^x \pm J_j^y$ should not generate confusion with angular momentum operators. [4]

Next, we switch to spinless fermions, since all terms appearing in the previous expression do not involve explicitly the non-linear string operator K_i. In terms of fermions, the Hamiltonian is essentially idential:

$$\hat{H} = -\sum_j \left[J_j^+ (\hat{c}_j^\dagger \hat{c}_{j+1} + H.c.) \, + \, J_j^- (\hat{c}_j^\dagger \hat{c}_{j+1}^\dagger + H.c.) \right] + \sum_j h_j (2\hat{n}_j - 1) \, ,$$

The only tricky point has to do with the boundary conditions. If one uses open boundary conditions, the first sum runs over $j = 1, \cdots, L-1$ and there is never a term involving site $L+1 \equiv 1$:

$$\hat{H}_{\rm OBC} = -\sum_{j=1}^{L-1} \left[J_j^+ (\hat{c}_j^\dagger \hat{c}_{j+1} + H.c.) \, + \, J_j^- (\hat{c}_j^\dagger \hat{c}_{j+1}^\dagger + H.c.) \right] + \sum_{j=1}^{L} h_j (2\hat{n}_j - 1) \, . \tag{1.12}$$

In the PBC-case, however, terms of the type $\hat{b}_L^\dagger \hat{b}_{L+1} \equiv \hat{b}_L^\dagger \hat{b}_1 = -(-1)^{N_F} \hat{c}_L^\dagger \hat{c}_1$ and $\hat{b}_L^\dagger \hat{b}_{L+1}^\dagger \equiv \hat{b}_L^\dagger \hat{b}_1^\dagger = -(-1)^{N_F} \hat{c}_L^\dagger \hat{c}_1^\dagger$ appear in the Hamiltonian, where N_F is the number of fermions. Therefore:

$$\hat{H}_{\rm PBC} = \hat{H}_{\rm OBC} + (-1)^{N_F} \left[J_L^+ (\hat{c}_L^\dagger \hat{c}_1 + H.c.) \, + \, J_L^- (\hat{c}_L^\dagger \hat{c}_1^\dagger + H.c.) \right] \, . \tag{1.13}$$

Notice that, although the number of fermions is in general *not conserved* by Hamiltonian of Eq.(1.13), the parity of N_F is conserved and $(-1)^{N_F}$ is a constant of the motion with value 1 or -1. So, we need to apply anti-periodic boundary conditions (ABC), $\hat{c}_{L+1} = -\hat{c}_1$, if there is an *even* number of fermions and periodic boundary condition (PBC), $\hat{c}_{L+1} = \hat{c}_1$, if there is an *odd* number of fermions.

As a warm up, let us study the ordered case.

1.3. Ordered Ising model.

In the ordered case, it is customary to take $J^x = J(1+\gamma)/2$ and $J^y = J(1-\gamma)/2$, so that $J^+ = J$ and $J^- = \gamma J$. The Hamiltonian is then:

$$\hat{H}_{\rm OBC} = -J \sum_{j=1}^{L-1} \left[(\hat{c}_j^\dagger \hat{c}_{j+1} + H.c.) \, + \, \gamma (\hat{c}_j^\dagger \hat{c}_{j+1}^\dagger + H.c.) \right] + h \sum_{j=1}^{L} (2\hat{c}_j^\dagger \hat{c}_j - 1) \, , \tag{1.14}$$

for the OBC case, and:

$$\hat{H}_{\rm PBC} = \hat{H}_{\rm OBC} + (-1)^{N_F} J \left[(\hat{c}_L^\dagger \hat{c}_1 + H.c.) \, + \, \gamma (\hat{c}_L^\dagger \hat{c}_1^\dagger + H.c.) \right] \, . \tag{1.15}$$

[4] Notice that there is no imaginary-i here: these are just real numbers.

[5] We assume, from now on, that the number of sites L is *even* (this is not a big restriction, and is useful). In the PBC case, if the number of fermions N_F is odd, then all J's are the same, and we can take $\hat{c}_{L+1} = \hat{c}_1$; if, on the contrary, N_F is even, then the L-th bond has an opposite sign to the remaining ones, which can also be reformulated as $\hat{c}_{L+1} = -\hat{c}_1$. Since the Hamiltonian conserves the fermion parity, both the even and the odd sector of the fermionic Hilbert space have to be considered when diagonalizing the model, i.e., $\hat{H} = \hat{H}^{\rm e} + \hat{H}^{\rm e}$, where $\hat{H}^{\rm e/o}$ denote the even/odd subspace restrictions. [6] Let us now introduce the fermion operators in k-space, $\hat{c}_k$ and $\hat{c}_k^\dagger$, so defined:

$$\begin{cases} \hat{c}_k &= \dfrac{{\rm e}^{-i\phi}}{\sqrt{L}} \displaystyle\sum_{j=1}^{L} {\rm e}^{-ikj} \hat{c}_j \\ \hat{c}_j &= \dfrac{{\rm e}^{i\phi}}{\sqrt{L}} \displaystyle\sum_{k} {\rm e}^{+ikj} \hat{c}_k \end{cases} , \tag{1.16}$$

where the overall phase ${\rm e}^{i\phi}$ is irrelevant for the canonical anticommutation relations, but might be useful to change the phase of the anomalous BCS pair-creation terms. In the following we will set $\phi = 0$, which will lead to the appearence of an i in the final Hamiltonian. Which values of k appear in the previous transformation *depends* on the boundary conditions. If N_F is odd we should take PBC for the fermions, which implies $\hat{c}_{L+1} = \hat{c}_1$: this in turn implies for the k's (from the expression for $\hat{c}_j$ in terms of $\hat{c}_k$) that ${\rm e}^{ikL} = 1$, i.e., the usual choice $k = \frac{2\pi n}{L}$, with $n = -\frac{L}{2} + 1, \cdots, \frac{L}{2}$ (since we assumed L even):

$$N_F \text{ odd} \iff \text{PBC} \implies k = \frac{2\pi n}{L} \quad \text{with} \quad n = -\frac{L}{2} + 1, \cdots, \frac{L}{2} \, . \tag{1.17}$$

If N_F is even, then we have to take ABC for the fermions, $\hat{c}_{L+1} = -\hat{c}_1$, which requires a different choice for the k's, leading to ${\rm e}^{ikL} = -1$: $k = \pm\frac{\pi(2n+1)}{L}$ with $n = 0, \cdots, \frac{L}{2} - 1$:

$$N_F \text{ even} \iff \text{ABC} \implies k = \pm\frac{\pi(2n+1)}{L} \quad \text{with} \quad n = 0, \cdots, \frac{L}{2} - 1 \, . \tag{1.18}$$

In terms of $\hat{c}_k$ and $\hat{c}_k^\dagger$, $\hat{H}^{\rm e/o}$ becomes (with the appropriate choice of the k-vectors):

$$\hat{H}^{\rm e/o} = -J \sum_k \Big[2\cos k \; \hat{c}_k^\dagger \hat{c}_k \; + \; \gamma \Big({\rm e}^{ik} \hat{c}_k^\dagger \hat{c}_{-k}^\dagger + H.c. \Big) \Big] + h \sum_k (2\hat{c}_k^\dagger \hat{c}_k - 1) \, . \tag{1.19}$$

Notice the coupling of $-k$ with k in the anomalous term, with the exceptions of $k = 0$ and $k = \pi$ for the PBC-case, which do not have a separate $-k$ partner. By grouping together terms with k and $-k$, the Hamiltonian is decoupled into a sum of independent terms acting

[5] Notice that one can change the sign of the h-term by making a particle-hole transformation $\tilde{c}_j \to (-1)^j \hat{c}_j^\dagger$, which transforms $\tilde{n}_j \to 1 - \hat{n}_j$, and $1 - 2\tilde{n}_j \to 2\hat{n}_j - 1$, while leaving the hopping term untouched (same sign of J). With the current choice of the h-term, the $h \to +\infty$ ground state in the spin representation $|\downarrow\downarrow \cdots \downarrow\rangle$ is mapped into the fermionic vacuum, which will be useful in discussing the ground state. (Notice that the phase factor $(-1)^j$ exchange the roles of $k = 0$ and $k = \pi$ in the discussion of the ground state.) Similarly, the same particle-hole transformation but without phase factor $(-1)^j$ would also invert the sign of the J-term, from ferromagnetic to antiferromagnetic.

[6] $\hat{H}^{\rm e/o}$ act on different subspaces, and we should more properly write them as $\hat{P}^{\rm e/o} \hat{H}^{\rm e/o} \hat{P}^{\rm e/o}$, in terms of projectors $\hat{P}^{\rm e/o}$ in the respective sectors.

in the 4-dimensional Hilbert spaces generated by k and $-k$:

$$\begin{aligned}\hat{H}^{\rm e} &= \sum_{k>0}^{\rm ABC} \hat{H}_k \\ \hat{H}^{\rm o} &= \sum_{k>0}^{\rm PBC} \hat{H}_k + \hat{H}_{k=0} + \hat{H}_{k=\pi}\end{aligned}$$

where we have singled-out $\hat{H}_{k=0} = -2(J-h)\hat{n}_0 - h$ and $H_{k=\pi} = 2(J+h)\hat{n}_\pi - h$ for the N_F-odd (PBC) case, and:

$$\hat{H}_k = -2J\left[\cos k\left(\hat{c}_k^\dagger \hat{c}_k - \hat{c}_{-k}\hat{c}_{-k}^\dagger\right) + i\gamma \sin k\left(\hat{c}_k^\dagger \hat{c}_{-k}^\dagger - \hat{c}_{-k}\hat{c}_k\right)\right] + 2h\left(\hat{c}_k^\dagger \hat{c}_k - \hat{c}_{-k}\hat{c}_{-k}^\dagger\right) .$$

Notice the transformation of the $\cos(-k)$ term, where we used $\sum_{k>0}\cos k = 0$, whose usefulness will be appreciated in a moment. Notice also that

$$(2\hat{c}_k^\dagger \hat{c}_k - 1) + (2\hat{c}_{-k}^\dagger \hat{c}_{-k} - 1) = 2(\hat{c}_k^\dagger \hat{c}_k - \hat{c}_{-k}\hat{c}_{-k}^\dagger) .$$

With the Nambu formalism, we define the fermionic two-component spinor

$$\widehat{\Psi}_k = \begin{pmatrix} \hat{c}_k \\ \hat{c}_{-k}^\dagger \end{pmatrix} , \qquad \widehat{\Psi}_k^\dagger = (\hat{c}_k^\dagger \ \hat{c}_{-k}) \tag{1.20}$$

with commutation relations ($\alpha = 1, 2$ stands for the two components of $\widehat{\Psi}$)

$$\{\widehat{\Psi}_{k\alpha}, \widehat{\Psi}_{k'\alpha'}^\dagger\} = \delta_{\alpha,\alpha'}\delta_{k,k'} . \tag{1.21}$$

We can then rewrite each $\hat{H}_k$ as:

$$\hat{H}_k = \sum_{\alpha,\beta} \widehat{\Psi}_{k\alpha}^\dagger \mathbb{H}_{\alpha\beta}^{(k)} \widehat{\Psi}_{k\beta} = (\hat{c}_k^\dagger \ \hat{c}_{-k}) \begin{pmatrix} -2J\cos k + 2h & -2i\gamma J \sin k \\ 2i\gamma J \sin k & 2J\cos k - 2h \end{pmatrix} \begin{pmatrix} \hat{c}_k \\ \hat{c}_{-k}^\dagger \end{pmatrix} . \tag{1.22}$$

Let us denote $\mathbb{H}_{11}^{(k)} = a_k = -2J\cos k + 2h$, and $\mathbb{H}_{12}^{(k)} = -ib_k$ with $b_k = 2\gamma J \sin k$, so that $\mathbb{H}^{(k)} = a_k\tau^z + b_k\tau^y$, with $\tau^{z,y}$ standard Pauli matrices (in Nambu space). By solving the 2×2 eigenvalue problem for $\mathbb{H}^{(k)}$ we find the eigenvalues $\epsilon_{k\pm} = \pm\epsilon_k$ with:

$$\epsilon_k = \sqrt{a_k^2 + b_k^2} = 2J\sqrt{\left(\cos k - \frac{h}{J}\right)^2 + \gamma^2 \sin^2 k} \tag{1.23}$$

with corresponding eigenvectors $(u_{k\pm} \ v_{k\pm})^T$. For the positive energy eigenvector, we have:

$$\begin{pmatrix} u_{k+} \\ v_{k+} \end{pmatrix} \equiv \begin{pmatrix} u_k \\ v_k \end{pmatrix} = \frac{1}{\sqrt{2\epsilon_k(\epsilon_k + a_k)}} \begin{pmatrix} \epsilon_k + a_k \\ ib_k \end{pmatrix} , \tag{1.24}$$

where we have introduced the shorthands $u_k = u_{k+}$ and $v_k = v_{k+}$. Note, in passing, that $u_{-k} = u_k$, while $v_{-k} = -v_k$, since b_k is odd. The negative-energy eigenvector $(u_{k-} \ v_{k-})^T$ is related to the previous one by a simple transformation. Indeed, write the eigenvalue problem for $\epsilon_{k+} = +\epsilon_k$:

$$\begin{cases} a_k u_k - ib_k v_k &= \epsilon_k u_k \\ ib_k u_k - a_k v_k &= \epsilon_k v_k \end{cases} . \tag{1.25}$$

Now change sign to the first equation, take the complex-conjugate of both, and rewrite them in inverted order, to get:

$$\left\{ \begin{array}{rcl} a_k(-v_k^*) - ib_k u_k^* & = -\epsilon_k(-v_k^*) = \epsilon_{k-}(-v_k^*) \\ ib_k(-v_k^*) - a_k u_k^* & = -\epsilon_k(\ u_k^*) = \epsilon_{k-}(u_k^*) \end{array} \right. , \tag{1.26}$$

which is the eigenvalue equation for $(u_{k-}\ v_{k-})^T$. Therefore:

$$\left(\begin{array}{c} u_{k-} \\ v_{k-} \end{array} \right) = \left(\begin{array}{c} -v_k^* \\ u_k^* \end{array} \right) = \frac{1}{\sqrt{2\epsilon_k(\epsilon_k + a_k)}} \left(\begin{array}{c} ib_k \\ \epsilon_k + a_k \end{array} \right) . \tag{1.27}$$

The unitary matrix $\mathbb{U}_k$ having the two previous eigenvectors as colums:

$$\mathbb{U}_k = \left(\begin{array}{cc} u_k & -v_k^* \\ v_k & u_k^* \end{array} \right) , \tag{1.28}$$

diagonalizes $\mathbb{H}^{(k)}$:

$$\mathbb{U}_k^\dagger\ \mathbb{H}^{(k)}\ \mathbb{U}_k = \mathrm{diag}(\epsilon_k, -\epsilon_k) . \tag{1.29}$$

So, define new fermion Nambu operators Φ_k through

$$\widehat{\Phi}_k = \mathbb{U}_k^\dagger \widehat{\Psi}_k = \left(\begin{array}{c} u_k^* \hat{c}_k + v_k^* \hat{c}_{-k}^\dagger \\ -v_k \hat{c}_k + u_k \hat{c}_{-k}^\dagger \end{array} \right) = \left(\begin{array}{c} \hat{\gamma}_k \\ \hat{\gamma}_{-k}^\dagger \end{array} \right) , \tag{1.30}$$

where, in the second term, we have made use of the fact that $u_{-k} = u_k$ and $v_{-k} = -v_k$. It is straightforward to verify that $\hat{\gamma}_k$ is indeed a fermion, i.e.

$$\begin{array}{rcl} \{\hat{\gamma}_k, \hat{\gamma}_k^\dagger\} & = & \{u_k^* \hat{c}_k + v_k^* \hat{c}_{-k}^\dagger, u_k \hat{c}_k^\dagger + v_k \hat{c}_{-k}\} \\ & = & |u_k|^2 \{\hat{c}_k, \hat{c}_k^\dagger\} + |v_k|^2 \{\hat{c}_{-k}^\dagger, \hat{c}_{-k}\} = |u_k|^2 + |v_k|^2 = 1 , \end{array} \tag{1.31}$$

the last equality following from the normalization condition for the eigenvectors. In terms of $\widehat{\Phi}_k = (\hat{\gamma}_k\ \hat{\gamma}_{-k}^\dagger)^T$ and $\widehat{\Phi}_k^\dagger = \widehat{\Psi}_k^\dagger \mathbb{U}_k = (\hat{\gamma}_k^\dagger\ \hat{\gamma}_{-k})$, we have:

$$\begin{array}{rcl} \hat{H}_k & = & \widehat{\Psi}_k^\dagger\ \mathbb{U}_k\ \mathbb{U}_k^\dagger\ \mathbb{H}^{(k)}\ \mathbb{U}_k\ \mathbb{U}_k^\dagger \widehat{\Psi}_k = \widehat{\Phi}_k^\dagger \left(\begin{array}{cc} \epsilon_k & 0 \\ 0 & -\epsilon_k \end{array} \right) \widehat{\Phi}_k = \epsilon_k \left(\hat{\gamma}_k^\dagger \hat{\gamma}_k - \hat{\gamma}_{-k} \hat{\gamma}_{-k}^\dagger \right) \\ & = & \epsilon_k \left(\hat{\gamma}_k^\dagger \hat{\gamma}_k + \hat{\gamma}_{-k}^\dagger \hat{\gamma}_{-k} - 1 \right) . \end{array} \tag{1.32}$$

The form of the two bands $\pm\epsilon_k$, as a function of k and for several values of h is noteworthy. Figs. 1.1-1.2 show some plots that illustrate them.

Equally amusing is to see the behaviour of the "effective magnetic field" $\mathbf{R}(k) = (0, b_k, a_k)$, of magnitude $|\mathbf{R}(k)| = \epsilon_k$, that the system "sees" as the wavevector k spans the Brillouin zone (BZ) $(-\pi, \pi]$: When $h > J$ the z-component $R_z(k) = a_k$ is always *positive*, while for $h < J$ positive and negative values of $R_z(k)$ are visited: as a consequence, the magnetic field *direction* $\hat{\mathbf{R}}(k) = \mathbf{R}/|\mathbf{R}|$ stays always close to the North pole in spin space for $h > J$, while the whole meridian connecting North and South pole is visited for $h < J$. Notice that $\hat{\mathbf{R}}(k)$ is *singular*, close to $k = 0.$ at the critical point $h_c = J$, because $|\mathbf{R}(k = 0)| = 0$.

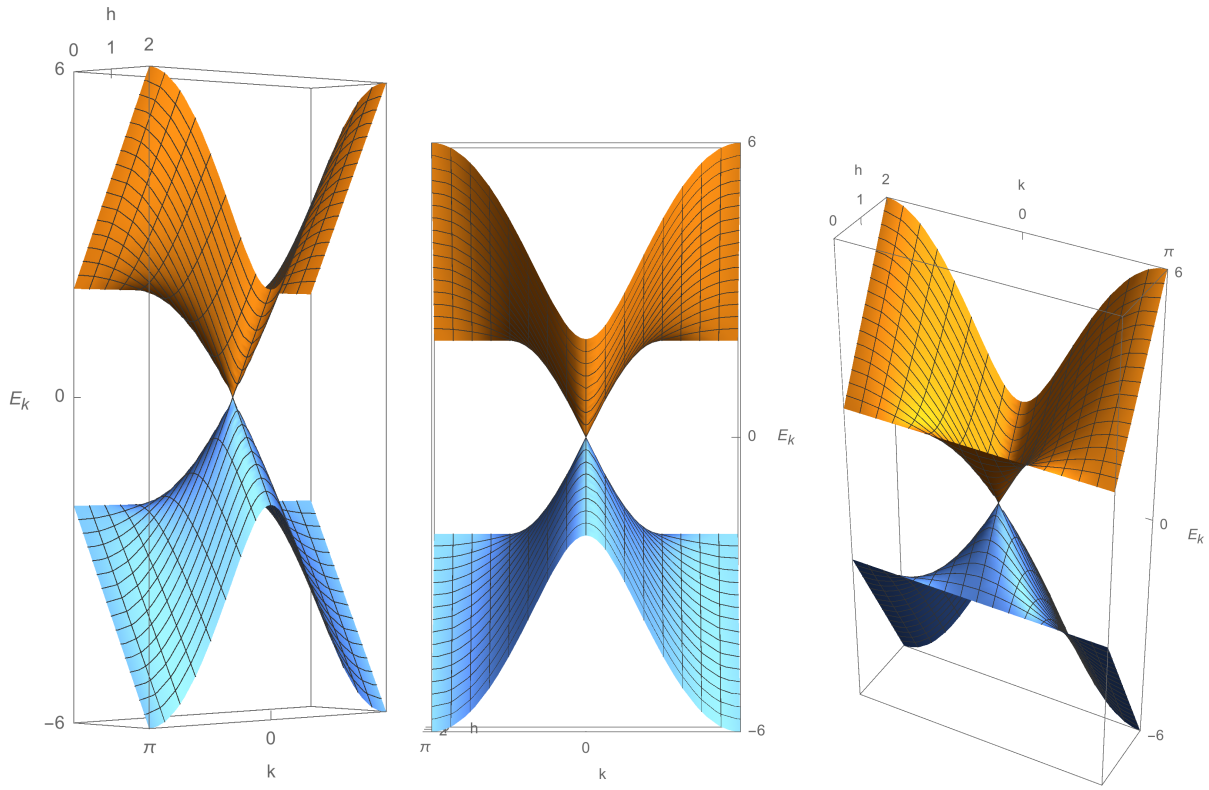

Figure 1.1.: The two bands $\pm\epsilon_k$ plotted by varying the transverse field h, seen from different viewpoints.

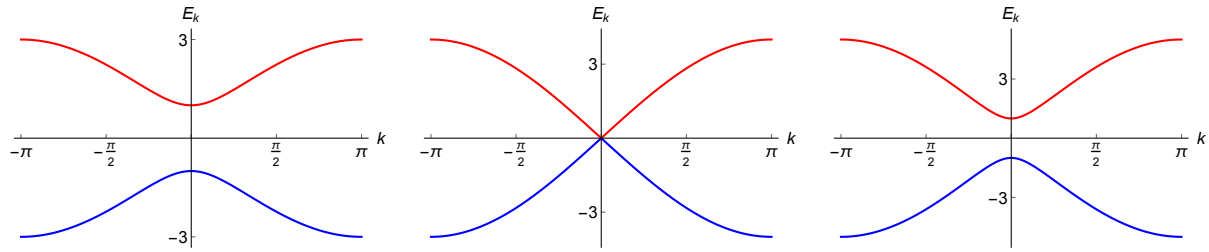

Figure 1.2.: The bands $\pm\epsilon_k$ for three different transverse fields h: $h/J = 0.5$ (left, inside the ferromagnetic region), $h/J = 1$ (center, the critical point), $h/J = 2$ (right, inside the paramagnetic phase). Notice the remarkable behaviour at $h = h_c = J$, clearly visible in the central panel: a gapless linear spectrum. Notice also how you can hardly distinguish the bands of the two gapped phases: but their topology is distinctly different (see text).

1.3.1. Ground state and lowest excited states of the Ising model.

The expression (1.32) allows to immediately conclude that the ground state of the Hamiltonian must be the state $|\emptyset\rangle_\gamma$ which annihilates the $\hat{\gamma}_k$ for all k — the so-called *Bogoliubov vacuum*:

$$\hat{\gamma}_k \, |\emptyset\rangle_\gamma = 0 \quad \forall k \; . \tag{1.33}$$

In principle, one can define two such states, one in the N_F-even (ABC) sector, and one in the N_F-odd (PBC). However, it is not very difficult to show [7] that the winner between the two, i.e., the actual global ground state, is the one in the N_F-even sector, with an energy

$$E_0^{\rm ABC} = -\sum_{k>0}^{\rm ABC} \epsilon_k \; . \tag{1.34}$$

The ground state can be obtained explicitly as:

$$|\emptyset\rangle_\gamma^{\rm ABC} \propto \prod_{k>0} \hat{\gamma}_{-k}\hat{\gamma}_k|0\rangle \tag{1.35}$$

where $|0\rangle$ is the vacuum for the original fermions, $\hat{c}_k|0\rangle = 0$. So

$$\begin{aligned} \prod_{k>0} \hat{\gamma}_{-k}\hat{\gamma}_k|0\rangle &= \prod_{k>0} \Big(u^*_{-k}\hat{c}_{-k} + v^*_{-k}\hat{c}^\dagger_k\Big)\Big(u^*_k\hat{c}_k + v^*_k\hat{c}^\dagger_{-k}\Big)|0\rangle \\ &= \prod_{k>0} v^*_k\Big(u^*_{-k} + v^*_{-k}\hat{c}^\dagger_k\hat{c}^\dagger_{-k}\Big)|0\rangle = \prod_{k>0} v^*_k\Big(u_k + v_k\hat{c}^\dagger_k\hat{c}^\dagger_{-k}\Big)|0\rangle \; , \end{aligned} \tag{1.36}$$

and by normalizing the state, we arrive at a standard BCS expression:

$$|\emptyset\rangle_\gamma^{\rm ABC} = \prod_{k>0}^{\rm ABC} \Big(u_k + v_k\hat{c}^\dagger_k\hat{c}^\dagger_{-k}\Big)|0\rangle \; . \tag{1.37}$$

The PBC-sector ground state must contain an *odd* number of particles. Since a BCS-paired state is always fermion-even, the unpaired Hamiltonian terms $\hat{H}_{k=0} + \hat{H}_{k=\pi}$ must contribute with exactly *one* fermion in the ground state. It is simple to verify that, with our choice of the sign of h, the ground state has $\hat{n}_{k=0} = 1$ and $\hat{n}_{k=\pi} = 0$, resulting in an extra term of the form $\delta E_{0,\pi} = \min(\hat{H}_0 + \hat{H}_\pi) = -2J$. The PBC-ground state is, therefore:

$$|\emptyset\rangle_\gamma^{\rm PBC} = \hat{c}^\dagger_{k=0} \prod_{0<k<\pi}^{\rm PBC} \Big(u_k + v_k\hat{c}^\dagger_k\hat{c}^\dagger_{-k}\Big)|0\rangle \; . \tag{1.38}$$

The corresponding energy is:

$$E_0^{\rm PBC} = \delta E_{0,\pi} - \sum_{0<k<\pi}^{\rm PBC} \epsilon_k \; . \tag{1.39}$$

And here come a very amusing subtelty of the *thermodynamic limit* $L \to \infty$. You would *naively* expect that, when you considers the *energy-per-site* $e_0 = E_0/L$, then the ground state energy should simply tend to *an integral*:

$$e_0 = -\lim_{L\to\infty} \frac{1}{L} \sum_{k>0}^{\rm ABC} \epsilon_k = -\int_0^\pi \frac{{\rm d}k}{2\pi} \, \epsilon_k \; . \tag{1.40}$$

[7] Explain.

It turns out that the whole subtelty is hidden in the way one treates the boundary points at 0 and π. If you refrain from being too cavalier with the $L \to \infty$ limit, you discover that the energy splitting $\Delta E_0 = E_0^{\rm PBC} - E_0^{\rm ABC}$ is, in the whole ferromagnetically ordered region $-J < h < J$, a quantity that goes to zero *exponentially fast* when $L \to \infty$: in other words, the two sectors ABC and PBC provide you the required *double degeneracy* of the ferromagnatic phase: you can see that easily for $h = 0$; less trivial, but true, for all $|h| < J$. On the contrary, ΔE_0 is *finite* in the quantum disordered regions $|h| > J$, and goes to zero like $1/L$ at the critical points $h_c = \pm J$.

Regarding the excited states, the situation is simple enough within the N_F-even (ABC) sector. Here excited states are obtained by applying an *even* number of $\hat\gamma_k^\dagger$ to $|\emptyset\rangle_{\rm ABC}$, each $\hat\gamma_k^\dagger$ costing an energy ϵ_k:

$$\begin{aligned} |\psi_{\{n_k\}}\rangle &= \prod_k^{\rm ABC} [\hat\gamma_k^\dagger]^{n_k} |\emptyset\rangle_\gamma^{\rm ABC} \qquad \text{with} \quad n_k = 0,1 \quad \text{and} \quad \sum_k^{\rm ABC} n_k = \text{even} \\ E_{\{n_k\}} &= E_0^{\rm ABC} + \sum_k^{\rm ABC} n_k \epsilon_k \, . \end{aligned} \tag{1.41}$$

In the N_F-odd (PBC) sector, some care must be exercised. One could apply an even number of $\gamma_k^\dagger$ to the ground state $|\emptyset\rangle_{\rm PBC}$, or, alternatively, remove the fermion from the $k = 0$ state and apply only an odd number of $\gamma_k^\dagger$'s.

Do a careful analysis of the spectrum. Discuss also the OBC case.

1.4. Nambu formalism: general disordered case

As we have seen, in the ordered case the Hamiltonian can be diagonalized by a Fourier transformation, reducing the problem to a collection of 2×2 "pseudo-spin-1/2" problems, followed by a Bogoliubov transformation, as first shown by Lieb, Schultz and Mattis [1]. In disordered case we can proceed in an analogous way, but we cannot reduce ourselves to 2×2 problems in a simple way. [8] By using the Nambu formalism, we define a column vector $\widehat{\mathbf{\Psi}}$ and its Hermitian conjugate row vector $\widehat{\mathbf{\Psi}}^\dagger$, each of length $2L$, by

$$\widehat{\mathbf{\Psi}} = \begin{pmatrix} \hat c_1 \\ \vdots \\ \hat c_L \\ \hat c_1^\dagger \\ \vdots \\ \hat c_L^\dagger \end{pmatrix} = \begin{pmatrix} \hat{\mathbf{c}} \\ \hat{\mathbf{c}}^\dagger \end{pmatrix} \qquad \widehat{\mathbf{\Psi}}^\dagger = \begin{pmatrix} \hat c_1^\dagger \cdots \hat c_L^\dagger \; \hat c_1 \cdots \hat c_L \end{pmatrix} = \begin{pmatrix} \hat{\mathbf{c}}^\dagger & \hat{\mathbf{c}} \end{pmatrix} , \tag{1.42}$$

[8] For the time-independent case, a theorem due to Bloch and Messiah guarantees that there is always an appropriate basis in which the problem reduces to 2×2 blocks, but this is not very useful if you are willing to tackle dynamical problems. See later on.

or $\widehat{\Psi}_j = \hat{c}_j$, $\widehat{\Psi}_{j+L} = \hat{c}_j^\dagger$ and $\widehat{\Psi}_j^\dagger = \hat{c}_j^\dagger$, $\widehat{\Psi}_{j+L}^\dagger = \hat{c}_j$ for $j \le L$. Notice that the $\widehat{\mathbf{\Psi}}$ satisfy quite standard fermionic anti-commutation relations

$$\{\widehat{\Psi}_j, \widehat{\Psi}_{j'}^\dagger\} = \delta_{j,j'} \ , \tag{1.43}$$

for $j, j' = 1, ..., 2L$, except that $\{\widehat{\Psi}_j, \widehat{\Psi}_{j+L}\} = 1$ for all $j \le L$, which brings about certain factors 2 in the Heisenberg's equations of motion (see later). In order to be prepared for the general time-dependent case, assume that the couplings appearing in the general Ising Hamiltonian are time-dependent, and rewrite $\hat{H}(t)$ as a general quadratic form [9] of $\widehat{\mathbf{\Psi}}$ as:

$$\hat{H}(t) = \widehat{\mathbf{\Psi}}^\dagger \cdot \mathbb{H}(t) \cdot \widehat{\mathbf{\Psi}} = \begin{pmatrix} \hat{\mathbf{c}}^\dagger & \hat{\mathbf{c}} \end{pmatrix} \begin{pmatrix} \mathbf{A}(t) & \mathbf{B}(t) \\ -\mathbf{B}^*(t) & -\mathbf{A}^*(t) \end{pmatrix} \begin{pmatrix} \hat{\mathbf{c}} \\ \hat{\mathbf{c}}^\dagger \end{pmatrix} . \tag{1.45}$$

For the general quadratic fermion Hamiltonian the $2L \times 2L$ matrix $\mathbb{H}$ should be Hermitean, and its $L \times L$ blocks $\mathbf{A}$ and $\mathbf{B}$ should be, respectively, Hermitean ($\mathbf{A} = \mathbf{A}^\dagger$) and anti-symmetric ($\mathbf{B} = -\mathbf{B}^T$). In the Ising case, where all couplings are real, $\mathbb{H}$ is a $2L \times 2L$ real symmetric matrix, $\mathbf{A}$ is real and symmetric ($\mathbf{A} = \mathbf{A}^* = \mathbf{A}^T$), and $\mathbf{B}$ is real and anti-symmetric ($\mathbf{B} = \mathbf{B}^* = -\mathbf{B}^T$) hence we can write:

$$\mathbb{H}(t) = \begin{pmatrix} \mathbf{A}(t) & \mathbf{B}(t) \\ -\mathbf{B}^*(t) & -\mathbf{A}^*(t) \end{pmatrix} \stackrel{\text{Ising}}{\longrightarrow} \begin{pmatrix} \mathbf{A}(t) & \mathbf{B}(t) \\ -\mathbf{B}(t) & -\mathbf{A}(t) \end{pmatrix} . \tag{1.46}$$

The structure of the two blocks $\mathbf{A}$ and $\mathbf{B}$ is given, in the Ising case (omitting any t-dependence), by:

$$\begin{cases} A_{j,j} = h_j \\ A_{j,j+1} = A_{j+1,j} = -\dfrac{J_j^+}{2} = -\dfrac{J_j}{2} \end{cases} \qquad \begin{cases} B_{j,j} = 0 \\ B_{j,j+1} = -B_{j+1,j} = -\dfrac{J_j^-}{2} = -\dfrac{\gamma J_j}{2} \end{cases} , \tag{1.47}$$

where we have assumed, once again, that $J_j^x = J_j(1+\gamma)/2$ and $J^y = J_j(1-\gamma)/2$. In the PBC-spin case, we have additional matrix elements

$$\begin{aligned} A_{L,1} &= A_{1,L} = (-1)^{N_F} \frac{J_L^+}{2} = (-1)^{N_F} \frac{J_L}{2} , \\ B_{L,1} &= -B_{1,L} = (-1)^{N_F} \frac{J_L^-}{2} = (-1)^{N_F} \frac{\gamma J_L}{2} \end{aligned} \tag{1.48}$$

depending on the fermion parity: $(-1)^{N_F} = +1$ for the ABC-fermion case ($\hat{c}_{L+1} = -\hat{c}_1$, corresponding to even N_F) and $(-1)^{N_F} = -1$ for the PBC-fermion case ($\hat{c}_{L+1} = \hat{c}_1$, corresponding to odd N_F).

[9] Indeed one can show that the most general quadratic form in the fermion operators

$$\hat{H} = \sum_{j'j} 2A_{j'j} \hat{c}_{j'}^\dagger \hat{c}_j + \sum_{jj'} \left(B_{j'j} \hat{c}_{j'}^\dagger \hat{c}_j^\dagger + B_{j'j}^* \hat{c}_j \hat{c}_{j'} \right) , \tag{1.44}$$

where $A_{j'j} = A_{jj'}^*$ ($\mathbf{A} = \mathbf{A}^\dagger$ is Hermitean) and $B_{jj'} = -B_{j'j}$ ($\mathbf{B} = -\mathbf{B}^T$ is anti-symmetric, because $\hat{c}_j \hat{c}_{j'}$ is anti-symmetric under exchange of the two operators, and any symmetric part of $\mathbf{B}$ would not contribute) has exactly the form given in Eq. (1.45), plus a constant term $\mathrm{Tr}\mathbf{A}$.

1.5. Diagonalization of $\mathbb{H}$ in the time-independent case.

We start considering the eigenvalue problem for a general Hermitean $2L \times 2L$ matrix showing the intrinsic particle-hole symmetry of the problem leads to the Bogoljoubov-de Gennes (BdG) equations.

1.5.1. The Bogoljoubov-de Gennes equations.

Let us consider the eigenvalue problem for a general Hermitean $2L \times 2L$ matrix $\mathbb{H}$ (for a fixed time t, which we omit, in case there is a t-dependence)

$$\mathbb{H} \cdot \begin{pmatrix} \mathbf{u}_\mu \\ \mathbf{v}_\mu \end{pmatrix} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B}^* & -\mathbf{A}^* \end{pmatrix} \cdot \begin{pmatrix} \mathbf{u}_\mu \\ \mathbf{v}_\mu \end{pmatrix} = \epsilon_\mu \begin{pmatrix} \mathbf{u}_\mu \\ \mathbf{v}_\mu \end{pmatrix} \tag{1.49}$$

where $\mathbf{u}, \mathbf{v}$ are L-dimensional vector and μ index refers to μ-th eigenvector. By explicitly writing the previous system, we find the so-called Bogoliubov-De Gennes equations:

$$\begin{cases} \mathbf{A} \cdot \mathbf{u}_\mu + \mathbf{B} \cdot \mathbf{v}_\mu = \epsilon_\mu \mathbf{u}_\mu \\ -\mathbf{B}^* \cdot \mathbf{u}_\mu - \mathbf{A}^* \cdot \mathbf{v}_\mu = \epsilon_\mu \mathbf{v}_\mu \end{cases} \tag{1.50}$$

We can see that if $(\mathbf{u}_\mu \ \mathbf{v}_\mu)^T$ is eigenvector with eigenvalue ϵ_μ, then $\left(\mathbf{v}_\mu^* \ \mathbf{u}_\mu^*\right)^T$ is an eigenvector with eigenvalue $-\epsilon_\mu$. Indeed:

$$\begin{cases} \mathbf{A} \cdot \mathbf{v}_\mu^* + \mathbf{B} \cdot \mathbf{u}_\mu^* = -\epsilon_\mu \mathbf{v}_\mu^* \\ -\mathbf{B}^* \cdot \mathbf{v}_\mu^* - \mathbf{A}^* \cdot \mathbf{u}_\mu^* = -\epsilon_\mu \mathbf{u}_\mu^* \end{cases} , \tag{1.51}$$

coincides exactly with Eq. (1.50), after taking a complex conjugation, exchanging the two equations and reshuffling the terms. In the Ising case, $\mathbf{A} = \mathbf{A}^*$ and $\mathbf{B} = \mathbf{B}^*$, and we can always take the solutions to be real. [10] We can organize eigenvectors in a unitary (orthogonal, if the solutions are real) $2L \times 2L$ matrix

$$\mathbb{U} = \left(\begin{array}{ccc|ccc} \mathbf{u}_1 & \cdots & \mathbf{u}_L & \mathbf{v}_1^* & \cdots & \mathbf{v}_L^* \\ \hline \mathbf{v}_1 & \cdots & \mathbf{v}_L & \mathbf{u}_1^* & \cdots & \mathbf{u}_L^* \end{array}\right) = \begin{pmatrix} \mathbf{U} & \mathbf{V}^* \\ \mathbf{V} & \mathbf{U}^* \end{pmatrix} \tag{1.52}$$

$\mathbf{U}$ and $\mathbf{V}$ being $L \times L$ matrices (real, as we can choose to be, in the Ising case) and so

$$\mathbb{U}^\dagger \cdot \mathbb{H} \cdot \mathbb{U} = \mathbb{E}_D = \mathrm{diag}(\epsilon_\mu, -\epsilon_\mu) \tag{1.53}$$

If we define new fermion [11] operators $\widehat{\mathbf{\Phi}}$ and $\widehat{\mathbf{\Phi}}^\dagger$ in such way that

$$\widehat{\mathbf{\Psi}} = \mathbb{U} \cdot \widehat{\mathbf{\Phi}} \tag{1.54}$$

[10] Since $\mathbb{H}$ is a real and symmetric matrix, it can can be diagonalized by a real orthogonal matrix.

[11] We have $\widehat{\Phi}_i = \sum_j \mathbb{U}_{ij}^\dagger \widehat{\Psi}_j$ and $\widehat{\Phi}_k^\dagger = \sum_j \widehat{\Psi}_j^\dagger \mathbb{U}_{jk}$, and so

$$\begin{aligned} \{\widehat{\Phi}_i, \widehat{\Phi}_k^\dagger\} &= \{\sum_{j'} \mathbb{U}_{ij'}^\dagger \widehat{\Psi}_{j'}, \sum_j \widehat{\Psi}_j^\dagger \mathbb{U}_{jk}\} = \sum_{jj'} \mathbb{U}_{ij'}^\dagger \mathbb{U}_{jk} \{\widehat{\Psi}_{j'}, \widehat{\Psi}_j^\dagger\} \\ &= \sum_j \mathbb{U}_{ij}^\dagger \mathbb{U}_{jk} = (\mathbb{U}^\dagger \mathbb{U})_{ik} = \delta_{ik} \end{aligned}$$

we can write $\hat{H}$ in diagonal form

$$\hat{H} = \widehat{\mathbf{\Psi}}^\dagger \cdot \mathbb{H} \cdot \widehat{\mathbf{\Psi}} = \widehat{\mathbf{\Phi}}^\dagger \cdot \mathbb{U}^\dagger \cdot \mathbb{H} \cdot \mathbb{U} \cdot \widehat{\mathbf{\Phi}} = \widehat{\mathbf{\Phi}}^\dagger \cdot \mathbb{E}_D \cdot \widehat{\mathbf{\Phi}} \ . \tag{1.55}$$

Similarly to $\widehat{\mathbf{\Psi}} = (\hat{\mathbf{c}} \ \ \hat{\mathbf{c}}^\dagger)^T$, we can define new fermion operators $\hat{\boldsymbol{\gamma}}$ such that $\widehat{\mathbf{\Phi}} = (\hat{\boldsymbol{\gamma}} \ \ \hat{\boldsymbol{\gamma}}^\dagger)^T$. By using the fact that

$$\widehat{\mathbf{\Phi}} = \begin{pmatrix} \hat{\boldsymbol{\gamma}} \\ \hat{\boldsymbol{\gamma}}^\dagger \end{pmatrix} = \mathbb{U}^\dagger \cdot \widehat{\mathbf{\Psi}} = \begin{pmatrix} \mathbf{U}^\dagger & \mathbf{V}^\dagger \\ \mathbf{V}^T & \mathbf{U}^T \end{pmatrix} \cdot \begin{pmatrix} \hat{\mathbf{c}} \\ \hat{\mathbf{c}}^\dagger \end{pmatrix} \tag{1.56}$$

we can write: [12]

$$\begin{cases} \hat{\gamma}_\mu &= \sum_{j=1}^{L} (U^*_{j\mu} \hat{c}_j + V^*_{j\mu} \hat{c}^\dagger_j) \\ \hat{\gamma}^\dagger_\mu &= \sum_{j=1}^{L} (V_{j\mu} \hat{c}_j + U_{j\mu} \hat{c}^\dagger_j) \end{cases} , \tag{1.59}$$

which can be easily inverted, remembering that $\widehat{\mathbf{\Psi}} = \mathbb{U} \cdot \widehat{\mathbf{\Phi}}$, to express the $\hat{c}_j$ operators in terms of the $\hat{\gamma}_\mu$:

$$\begin{cases} \hat{c}_j &= \sum_{\mu} (U_{j\mu} \hat{\gamma}_\mu + V^*_{j\mu} \hat{\gamma}^\dagger_\mu) \\ \hat{c}^\dagger_j &= \sum_{\mu} (V_{j\mu} \hat{\gamma}_\mu + U^*_{j\mu} \hat{\gamma}^\dagger_\mu) \end{cases} . \tag{1.60}$$

Finally $\hat{H}$ in terms of the $\hat{\boldsymbol{\gamma}}$ operators reads, assuming we have taken $\epsilon_\mu > 0$:

$$\hat{H} = \sum_{\mu=1}^{L} \left(\epsilon_\mu \hat{\gamma}^\dagger_\mu \hat{\gamma}_\mu - \epsilon_\mu \hat{\gamma}_\mu \hat{\gamma}^\dagger_\mu \right) = \sum_{\mu=1}^{L} 2\epsilon_\mu \left(\hat{\gamma}^\dagger_\mu \hat{\gamma}_\mu - \frac{1}{2} \right) \tag{1.61}$$

and the ground state is the state annihilated by all $\hat{\gamma}_\mu$, we denote it by $|\emptyset\rangle_\gamma$ with $\hat{\gamma}_\mu \ |\emptyset\rangle_\gamma$, whose energy is

$$E_0 = -\sum_{\mu=1}^{L} \epsilon_\mu \ . \tag{1.62}$$

Once again, the excited states can be expressed as:

$$\begin{aligned} |\psi_{\{n_\mu\}}\rangle &= \prod_\mu [\hat{\gamma}^\dagger_\mu]^{n_\mu} |\emptyset\rangle_\gamma \qquad \text{with} \quad n_\mu = 0, 1 \\ E_{\{n_\mu\}} &= E_0 + 2 \sum_\mu n_\mu \epsilon_\mu \ , \end{aligned} \tag{1.63}$$

[12] The conditions for the transformation in Eq. (1.59) to be canonical are:

$$\mathbb{U}^\dagger \cdot \mathbb{U} = \left[\begin{array}{c|c} \mathbf{U}^\dagger \cdot \mathbf{U} + \mathbf{V}^\dagger \cdot \mathbf{V} & \mathbf{U}^\dagger \cdot \mathbf{V}^* + \mathbf{V}^\dagger \cdot \mathbf{U}^* \\ \hline \mathbf{V}^T \cdot \mathbf{U} + \mathbf{U}^T \cdot \mathbf{V} & \mathbf{V}^T \cdot \mathbf{V}^* + \mathbf{U}^T \cdot \mathbf{U}^* \end{array} \right] = \left[\begin{array}{c|c} \mathbf{1} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{1} \end{array} \right] \quad \Rightarrow \quad \begin{cases} \mathbf{U}^\dagger \cdot \mathbf{U} + \mathbf{V}^\dagger \cdot \mathbf{V} = \mathbf{1} \\ \mathbf{V}^T \cdot \mathbf{U} + \mathbf{U}^T \cdot \mathbf{V} = \mathbf{0} \end{cases} \tag{1.57}$$

since you realize that the block 22 is simply the $*$ of block 11 and block 12 is the $\dagger$ of block 21. Similarly, one must have:

$$\mathbb{U} \cdot \mathbb{U}^\dagger = \left[\begin{array}{c|c} \mathbf{U} \cdot \mathbf{U}^\dagger + \mathbf{V}^* \cdot \mathbf{V}^T & \mathbf{U} \cdot \mathbf{V}^\dagger + \mathbf{V}^* \cdot \mathbf{U}^T \\ \hline \mathbf{V} \cdot \mathbf{U}^\dagger + \mathbf{U}^* \cdot \mathbf{V}^T & \mathbf{V} \cdot \mathbf{V}^\dagger + \mathbf{U}^* \cdot \mathbf{U}^T \end{array} \right] = \left[\begin{array}{c|c} \mathbf{1} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{1} \end{array} \right] \quad \Rightarrow \quad \begin{cases} \mathbf{U} \cdot \mathbf{U}^\dagger + \mathbf{V}^* \cdot \mathbf{V}^T = \mathbf{1} \\ \mathbf{U} \cdot \mathbf{V}^\dagger + \mathbf{V}^* \cdot \mathbf{U}^T = \mathbf{0} \end{cases} \tag{1.58}$$

with the usual care on the parity of the number of fermions, in case the boundary conditions are not open.

1.5.2. The BCS-form of the ground state.

The next problem we would like to solve is how to write the Bogoliubov vacuum $|\emptyset\rangle_\gamma$ in terms of the $\hat{c}_j^\dagger$ in the general non-homogeneous case, in a way that generalizes the simple BCS form we have in k-space:

$$|\emptyset\rangle_\gamma^{\rm ABC} = \prod_{k>0}^{\rm ABC} \Big(u_k + v_k \hat{c}_k^\dagger \hat{c}_{-k}^\dagger \Big) |0\rangle \ . \tag{1.64}$$

For that purpose, let us make the *Ansatz* that $|\emptyset\rangle_\gamma$ can be written as a Gaussian state of the form:

$$|\emptyset\rangle_\gamma = \mathcal{N}\, {\rm e}^{\mathcal{Z}}\, |0\rangle = \mathcal{N}\, {\rm e}^{\frac{1}{2}(\hat{\mathbf{c}}^\dagger)^T \cdot \mathbf{Z} \cdot (\hat{\mathbf{c}}^\dagger)}\, |0\rangle = \mathcal{N}\, \exp\Big(\frac{1}{2} \sum_{j_1 j_2} Z_{j_1 j_2} \hat{c}_{j_1}^\dagger \hat{c}_{j_2}^\dagger \Big)\, |0\rangle \ , \tag{1.65}$$

where $\mathcal{Z}$ will be our shorthand notation for the quadratic fermion form we exponentiate. Clearly, since $\hat{c}_{j_1}^\dagger \hat{c}_{j_2}^\dagger = -\hat{c}_{j_2}^\dagger \hat{c}_{j_1}^\dagger$ we can take the matrix $\mathbf{Z}$ to be *antisymmetric* (but complex, in general): any symmetric part of $\mathbf{Z}$ would give 0 contribution. The conditions that $\mathbf{Z}$ has to satisfy should be inferred from the fact that we pretend that, $\forall \mu$, we must have $\hat{\gamma}_\mu |\emptyset\rangle_\gamma = 0$, which read:

$$\mathcal{N} \sum_{j=1}^{L} \Big(U_{j\mu}^* \hat{c}_j + V_{j\mu}^* \hat{c}_j^\dagger \Big)\, {\rm e}^{\mathcal{Z}}\, |0\rangle = 0 \qquad \forall \mu \ . \tag{1.66}$$

Since $\mathcal{Z}$ is made of *pairs* of $\hat{c}^\dagger$s, it commutes with $\hat{c}_j^\dagger$, hence, $\hat{c}_j^\dagger {\rm e}^{\mathcal{Z}} |0\rangle = {\rm e}^{\mathcal{Z}} \hat{c}_j^\dagger |0\rangle$. The first term, containing $\hat{c}_j {\rm e}^{\mathcal{Z}} |0\rangle$, is more problematic. We would like to commute $\hat{c}_j$ through ${\rm e}^{\mathcal{Z}}$ to bring it towards the $|0\rangle$, where it annihilates. To do so, let us start calculating:

$$\Big[\hat{c}_j, \mathcal{Z} \Big] = \frac{1}{2} \left[\hat{c}_j, \sum_{j_1 j_2} Z_{j_1 j_2} \hat{c}_{j_1}^\dagger \hat{c}_{j_2}^\dagger \right] = \sum_{j'} Z_{j j'} \hat{c}_{j'}^\dagger \ , \tag{1.67}$$

where we have used the antisymmetry of $\mathbf{Z}$. We see, therefore, that $[\hat{c}_j, \mathcal{Z}]$, being a combination of $\hat{c}_{j'}^\dagger$ commutes with $\mathcal{Z}$ and with any function of $\mathcal{Z}$. It takes then little algebra [13] to show that:

$$\Big[\hat{c}_j, {\rm e}^{\mathcal{Z}} \Big] = \Big[\hat{c}_j, \mathcal{Z} \Big]\, {\rm e}^{\mathcal{Z}} = {\rm e}^{\mathcal{Z}} \Big[\hat{c}_j, \mathcal{Z} \Big] \quad \Rightarrow \quad \hat{c}_j {\rm e}^{\mathcal{Z}} = {\rm e}^{\mathcal{Z}} \Big(\hat{c}_j + [\hat{c}_j, \mathcal{Z}] \Big) \ . \tag{1.68}$$

The conditions in Eq. (1.66) therefore read:

$$\mathcal{N}\, {\rm e}^{\mathcal{Z}} \sum_{j=1}^{L} \Big[U_{j\mu}^* \Big(\hat{c}_j + [\hat{c}_j, \mathcal{Z}] \Big) + V_{j\mu}^* \hat{c}_j^\dagger \Big]\, |0\rangle = 0 \qquad \forall \mu \ . \tag{1.69}$$

[13] Simply expand the exponential in the usual way, realize that

$$[\hat{c}_j, \mathcal{Z}^n] = n\, [\hat{c}_j, \mathcal{Z}]\, \mathcal{Z}^{n-1} \ ,$$

because $[\hat{c}_j, \mathcal{Z}]$ commutes with all powers of $\mathcal{Z}$, and reconstruct the exponential to get the result.

Noticing that $\hat{c}_j|0\rangle = 0$, substituting Eq. (1.67), and omitting irrelevant prefactors we therefore have:

$$\Big[\sum_{jj'} U^*_{j'\mu} Z_{j'j} \hat{c}^\dagger_j + \sum_j V^*_{j\mu} \hat{c}^\dagger_j\Big]\,|0\rangle = 0 \qquad \forall \mu\ , \tag{1.70}$$

where we have exchanged the dummy indices j and j' in the first term. Next, we collect the two terms by writing:

$$\sum_j \Big[(\mathbf{U}^\dagger \cdot \mathbf{Z})_{\mu j} + (\mathbf{V}^\dagger)_{\mu j}\Big]\,\hat{c}^\dagger_j\,|0\rangle = 0 \quad \Rightarrow \quad \mathbf{Z} = -(\mathbf{U}^\dagger)^{-1} \cdot \mathbf{V}^\dagger\ . \tag{1.71}$$

This is the condition that $\mathbf{Z}$ has to verify in order for the state $|\emptyset\rangle_\gamma$ to be annihilated by all $\hat{\gamma}_\mu$. This is the so-called *Thouless formula*. It takes very little algebra [14] to verify that, indeed, such a form of $\mathbf{Z}$ is *antisymmetric*.

According to a theorem of linear algebra, an antisymmetric matrix can always be reduced to a "standard canonical" form by applying a unitary matrix $\mathbf{D}$ as follows:

$$\mathbf{Z} = \mathbf{D} \cdot \mathbf{\Lambda} \cdot \mathbf{D}^T \qquad \text{with} \qquad \mathbf{\Lambda} = \left[\begin{array}{cc|cc|c} 0 & \lambda_1 & 0 & 0 & \cdots \\ -\lambda_1 & 0 & 0 & 0 & \cdots \\ \hline 0 & 0 & 0 & \lambda_2 & \cdots \\ 0 & 0 & -\lambda_2 & 0 & \cdots \\ \hline \vdots & \vdots & \vdots & \vdots & \vdots \end{array}\right]_{L\times L}\ , \tag{1.73}$$

where in general the λ_p are complex. If L is *even*, there are $\frac{L}{2}$ blocks 2×2 with some λ_p, while if L is *odd*, Λ has an extra row/column of zeroes. The unitary matrix $\mathbf{D}$ allows us to define combinations of the fermions $c^\dagger_j$ which form natural "BCS-paired" orbitals,

$$\hat{d}^\dagger_p = \sum_j (\mathbf{D}^T)_{pj} \hat{c}^\dagger_j = \sum_j D_{jp} \hat{c}^\dagger_j\ . \tag{1.74}$$

Labelling the consecutive columns of $\mathbf{D}$ as $1, \overline{1}, 2, \overline{2}, \cdots, p, \overline{p}, \cdots$, with p up to $L/2$, one can readily check that in terms of the $d^\dagger$s the Bogoliubov vacuum $|\emptyset\rangle_\gamma$ reads:

$$|\emptyset\rangle_\gamma = \mathcal{N}\ \exp\Big(\sum_{p=1}^{L/2} \lambda_p \hat{d}^\dagger_p \hat{d}^\dagger_{\overline{p}}\Big)\,|0\rangle = \mathcal{N} \prod_{p=1}^{L/2} \Big(1 + \lambda_p \hat{d}^\dagger_p \hat{d}^\dagger_{\overline{p}}\Big)\,|0\rangle\ . \tag{1.75}$$

[14] Observe that:

$$\mathbf{Z}^T = -(\mathbf{V}^\dagger)^T \cdot \Big((\mathbf{U}^\dagger)^{-1}\Big)^T = -\mathbf{V}^* \cdot \Big((\mathbf{U}^\dagger)^T\Big)^{-1} = -\mathbf{V}^* \cdot (\mathbf{U}^*)^{-1}\ .$$

However, from block 12 in Eq. (1.57) we get:

$$\mathbf{U}^\dagger \cdot \mathbf{V}^* = -\mathbf{V}^\dagger \cdot \mathbf{U}^* \quad \Rightarrow \quad \mathbf{Z}^T = -\mathbf{V}^* \cdot (\mathbf{U}^*)^{-1} = (\mathbf{U}^\dagger)^{-1} \cdot \mathbf{V}^\dagger = -\mathbf{Z}\ . \tag{1.72}$$

It remains to evaluate the normalization constant $\mathcal{N}$. Now we calculate: [15]

$$
\begin{aligned}
1 = {}_\gamma\langle\emptyset|\emptyset\rangle_\gamma &= |\mathcal{N}|^2 \, \langle 0| \prod_{p=1}^{L/2} \left(1 + \lambda_p^* \hat{d}_{\overline{p}} \hat{d}_p\right) \left(1 + \lambda_p \hat{d}_p^\dagger \hat{d}_{\overline{p}}^\dagger\right) |0\rangle \\
&= |\mathcal{N}|^2 \prod_{p=1}^{L/2} \left(1 + |\lambda_p|^2\right) = |\mathcal{N}|^2 \left[\det\left(\mathbf{1} + \mathbf{\Lambda} \cdot \mathbf{\Lambda}^\dagger\right)\right]^{1/2} = |\mathcal{N}|^2 \left[\det\left(\mathbf{1} + \mathbf{Z} \cdot \mathbf{Z}^\dagger\right)\right]^{1/2} \\
&= |\mathcal{N}|^2 \left[\det\left(\mathbf{1} + (\mathbf{U}^\dagger)^{-1} \cdot \mathbf{V}^\dagger \cdot \mathbf{V} \cdot \mathbf{U}^{-1}\right)\right]^{1/2} \\
&= |\mathcal{N}|^2 \left[\det\left((\mathbf{U}^\dagger)^{-1} \cdot (\mathbf{U}^\dagger \cdot \mathbf{U} + \mathbf{V}^\dagger \cdot \mathbf{V}) \cdot \mathbf{U}^{-1}\right)\right]^{1/2} = |\mathcal{N}|^2 \left[\det\left((\mathbf{U} \cdot \mathbf{U}^\dagger)^{-1}\right)\right]^{1/2} \\
&= |\mathcal{N}|^2 \, \frac{1}{|\det[\mathbf{U}]|} \qquad \Rightarrow \qquad |\mathcal{N}| = \sqrt{|\det[\mathbf{U}]|} \, . \qquad (1.76)
\end{aligned}
$$

Summarizing, we have derived the so-called *Onishi formula*, which states that:

$$
\left|\langle 0|\emptyset\rangle_\gamma\right|^2 = |\mathcal{N}|^2 = |\det[\mathbf{U}]| \, . \qquad (1.77)
$$

If we express the Bogoljoubov vacuum in terms of the λ_p we have:

$$
|\emptyset\rangle_\gamma = \prod_{p=1}^{L/2} \frac{1}{\sqrt{1 + |\lambda_p|^2}} \left(1 + \lambda_p \hat{d}_p^\dagger \hat{d}_{\overline{p}}^\dagger\right) |0\rangle = \prod_{p=1}^{L/2} \left(u_p + v_p \hat{d}_p^\dagger \hat{d}_{\overline{p}}^\dagger\right) |0\rangle \, , \qquad (1.78)
$$

where we have defined $u_p = 1/\sqrt{1 + |\lambda_p|^2}$ and $v_p = \lambda_p / \sqrt{1 + |\lambda_p|^2}$, which verify $|u_p|^2 + |v_p|^2 = 1$.

1.6. Dynamics in the time-dependent case

A time-dependence can come from many different sources. The simplest case, which is used in the so-called *quantum annealing* approach, consists in assuming that the transverse fields are time-dependent $h_j(t)$, for instance they might be slowly annealed from a very large negative value towards zero:

$$
h_j \to h_j(t) = \frac{t}{\tau_Q} h_j \qquad (1.79)
$$

with $t \in (-\infty, 0]$, or changed in some periodic fashion. In this way the diagonal elements of matrix $\mathbf{A}$ become time dependent and consequently $\hat{H} \to \hat{H}(t)$. Alternatively, a time-dependence is found from doing time-dependent mean-field approaches. We proceed now in general, assuming $\mathbf{A}(t)$ and $\mathbf{B}(t)$.

[15] In the derivation we use that:

$$
\mathbf{\Lambda} \cdot \mathbf{\Lambda}^\dagger = \left[\begin{array}{cc|cc|c} |\lambda_1|^2 & 0 & 0 & 0 & \cdots \\ 0 & |\lambda_1|^2 & 0 & 0 & \cdots \\ \hline 0 & 0 & |\lambda_2|^2 & 0 & \cdots \\ 0 & 0 & 0 & |\lambda_2|^2 & \cdots \\ \hline \vdots & \vdots & \vdots & \vdots & \vdots \end{array}\right]_{L \times L} ,
$$

Start from Schrödinger's equation:

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle \ . \tag{1.80}$$

Since the norm of $|\psi(t)\rangle$ must be conserved, this implies the existence of a unitary evolution operator $\hat{U}(t,t_0)$ such that

$$|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle \ . \tag{1.81}$$

Therefore:

$$i\hbar\frac{d}{dt}\hat{U}(t,t_0)|\psi(t_0)\rangle = \hat{H}(t)\hat{U}(t,t_0)|\psi(t_0)\rangle \quad \forall|\psi(t_0)\rangle$$

$$\Rightarrow \quad i\hbar\frac{d}{dt}\hat{U}(t,t_0) = \hat{H}(t)\hat{U}(t,t_0) \ . \tag{1.82}$$

Next, consider the expectation value of a time-dependent operator $\hat{O}(t)$ in the Schrödinger's picture

$$\begin{aligned}\langle\hat{O}(t)\rangle \equiv \langle\psi(t)|\hat{O}(t)|\psi(t)\rangle &= \langle\psi(t_0)|\hat{U}^\dagger(t,t_0)\hat{O}(t)\hat{U}(t,t_0)|\psi(t_0)\rangle \\ &\equiv \langle\psi(t_0)|\hat{O}_H(t)|\psi(t_0)\rangle \ ,\end{aligned} \tag{1.83}$$

where we have introduced the Heisenberg's picture

$$\hat{O}_H(t) \equiv \hat{U}^\dagger(t,t_0)\hat{O}(t)\hat{U}(t,t_0) \ . \tag{1.84}$$

Therefore the equation of motion of an operator in Heisenberg's picture for the general case of a time-dependent Hamiltonian reads: [16]

$$i\hbar\frac{d}{dt}\hat{O}_H(t) = \hat{U}^\dagger(t,t_0)\left(\left[\hat{O}(t),\hat{H}(t)\right] + i\hbar\frac{\partial}{\partial t}\hat{O}(t)\right)\hat{U}(t,t_0) \tag{1.86}$$

1.6.1. The time-dependent Bogoljoubov-de Gennes equations.

Let's write the Heisenberg's equation of motion for operator $\hat{c}_j$

$$i\hbar\frac{d}{dt}\hat{c}_{jH}(t) = \hat{U}^\dagger(t,t_0)\left[\hat{c}_j,\hat{H}(t)\right]\hat{U}(t,t_0) \tag{1.87}$$

[16] Here we use:

$$i\hbar\frac{d}{dt}\hat{U}(t,t_0) = \hat{H}(t)\hat{U}(t,t_0) \quad \text{and} \quad -i\hbar\frac{d}{dt}\hat{U}^\dagger(t,t_0) = \hat{U}^\dagger(t,t_0)\hat{H}(t) \ .$$

Notice that if $\hat{H}$ and $\hat{O}$ are time independent

$$\left[\hat{U},\hat{H}\right] = \left[\hat{U}^\dagger,\hat{H}\right] = 0 \quad \text{and} \quad i\hbar\frac{\partial}{\partial t}\hat{O} = 0 \ ,$$

then Eq. (1.86) takes the well known form:

$$i\hbar\frac{d}{dt}\hat{O}_H = \left[\hat{O}_H,\hat{H}\right] \ . \tag{1.85}$$

By calculating the commutator

$$\begin{aligned}\left[\hat{c}_j, \hat{H}(t)\right] &= \sum_{\alpha,\beta=1}^{2L} \mathbb{H}_{\alpha\beta}(t) \left[\hat{c}_j, \widehat{\Psi}^\dagger_\alpha \widehat{\Psi}_\beta\right] \\ &= \sum_{\alpha,\beta=1}^{2L} \mathbb{H}_{\alpha\beta}(t) \left(\left\{\hat{c}_j, \widehat{\Psi}^\dagger_\alpha\right\} \widehat{\Psi}_\beta - \widehat{\Psi}^\dagger_\alpha \left\{\hat{c}_j, \widehat{\Psi}_\beta\right\}\right) \\ &= \sum_{\alpha,\beta=1}^{2L} \mathbb{H}_{\alpha\beta}(t) \left(\delta_{\alpha,j} \widehat{\Psi}_\beta - \widehat{\Psi}^\dagger_\alpha \delta_{\beta,j+L}\right) \\ &= 2\sum_{j'=1}^{L} \left[A_{jj'}(t)\hat{c}_{j'} + B_{jj'}(t)\hat{c}^\dagger_{j'}\right] \end{aligned} \tag{1.88}$$

we see that we have a *linear* equation of motion

$$i\hbar \frac{d}{dt}\hat{c}_{jH}(t) = 2\sum_{j'=1}^{L} \left[A_{jj'}(t)\ \hat{c}_{j'H}(t) + B_{jj'}(t)\ \hat{c}^\dagger_{j'H}(t)\right] \tag{1.89}$$

and analogously for the operator $\hat{c}^\dagger_j$. With a more compact notation, one can write the linear Heisenberg equations of motion for the elementary fermionic operators as:

$$i\hbar \frac{d}{dt}\widehat{\mathbf{\Psi}}_H(t) = 2\ \mathbb{H}(t) \cdot \widehat{\mathbf{\Psi}}_H(t)\ , \tag{1.90}$$

the factor 2 on the right-hand side originating from the off-diagonal $\{\widehat{\Psi}_j, \widehat{\Psi}_{j+L}\} = 1$. The initial condition for these equations can be written as:

$$\widehat{\mathbf{\Psi}}_H(t = t_0) \equiv \widehat{\mathbf{\Psi}}\ = \mathbb{U}_0 \cdot \begin{pmatrix} \hat{\boldsymbol{\gamma}} \\ \hat{\boldsymbol{\gamma}}^\dagger \end{pmatrix}\ , \tag{1.91}$$

where $\hat{\boldsymbol{\gamma}}$ are the Bogoljubov fermions that diagonalize $\hat{H}(t_0)$, and $\mathbb{U}_0$ the corresponding rotation matrix.

We are not quite done: We have an explicit linear equation for $\widehat{\mathbf{\Psi}}_H(t)$, but we need an *explicit solution* for this equation, obtained by some "simple enough" integration of a finite-dimensional linear problem.

There are now at least two ways of getting the desired result. Historically, the first one I was aware of runs roughly as follows.

First route. We make the *Ansatz* that $|\psi(t)\rangle$, the time-evolved state of the system, is a *Bogoliubov vacuum* annihilated by a set of *time-dependent* quasi-particle annihilation operators $\hat{\gamma}_\mu(t)$

$$\hat{\gamma}_\mu(t)\ |\psi(t)\rangle = 0 \qquad \forall\mu \quad \forall t\ . \tag{1.92}$$

This requirement immediately implies, by taking a total time-derivative, that:

$$\begin{aligned} 0 &= i\hbar\frac{d}{dt}\Big(\hat{\gamma}_\mu(t)\ |\psi(t)\rangle\Big) \\ &= \left(i\hbar\frac{\partial}{\partial t}\hat{\gamma}_\mu(t)\right)\ |\psi(t)\rangle + \hat{\gamma}_\mu(t)\left(i\hbar\frac{d}{dt}|\psi(t)\rangle\right) \\ &= \left(i\hbar\frac{\partial}{\partial t}\hat{\gamma}_\mu(t) + \hat{\gamma}_\mu(t)\hat{H}(t) - \hat{H}(t)\hat{\gamma}_\mu(t)\right)\ |\psi(t)\rangle \end{aligned} \tag{1.93}$$

where we have added, in the last step, a term $\hat{\gamma}_\mu(t)\,|\psi(t)\rangle = 0$. In turn, this last expression implies: [17]

$$i\hbar\frac{\partial}{\partial t}\hat{\gamma}_\mu(t) = -\left[\hat{\gamma}_\mu(t), \hat{H}(t)\right] \ . \tag{1.94}$$

By considering the equation of motion of the Heisenberg operator $\hat{\gamma}_{\mu H}(t)$ we have

$$i\hbar\frac{d}{dt}\hat{\gamma}_{\mu H}(t) = \hat{U}^\dagger(t,t_0)\left(\left[\hat{\gamma}_\mu(t), \hat{H}(t)\right] + i\hbar\frac{\partial}{\partial t}\hat{\gamma}_\mu(t)\right)\hat{U}(t,t_0) \equiv 0 \ , \tag{1.95}$$

where we have used Eq.1.94 in the last step. So, since $\hat{\gamma}_{\mu H}$ does not depend on t, it must coincide with its $t = t_0$ value; let's call this value $\hat{\gamma}_\mu = \hat{\gamma}_{\mu H} = \hat{\gamma}_\mu(t = t_0)$.

Let us assume now, inspired by Eq. (1.60), that the $\hat{c}_{jH}(t)$ are indeed expressed by

$$\hat{c}_{jH}(t) = \sum_{\mu=1}^{L}\left(U_{j\mu}(t)\ \hat{\gamma}_\mu + V^*_{j\mu}(t)\ \hat{\gamma}^\dagger_\mu\right) , \tag{1.96}$$

and let us see if this expression solves the required Heisenberg equations in Eq. (1.89) for an appropriate choice of the time-dependent coefficients $U_{j\mu}(t)$ and $V_{j\mu}(t)$. Substituting in Eq. (1.89) we get:

$$\begin{aligned}\sum_{\mu=1}^{L}\left[i\hbar\left(\frac{d}{dt}U_{j\mu}(t)\right)\hat{\gamma}_\mu + i\hbar\left(\frac{d}{dt}V^*_{j\mu}(t)\right)\hat{\gamma}^\dagger_\mu\right] &= 2\sum_{j=1}^{L}A_{ij}(t)\left[U_{j\mu}(t)\hat{\gamma}_\mu + V^*_{j\mu}(t)\hat{\gamma}^\dagger_\mu\right] \\ &+ 2\sum_{j=1}^{L}B_{ij}(t)\left[V_{j\mu}(t)\hat{\gamma}_\mu + U^*_{j\mu}(t)\hat{\gamma}^\dagger_\mu\right]\end{aligned} \tag{1.97}$$

By equating the coefficients of $\hat{\gamma}_\mu$ and $\hat{\gamma}^\dagger_\mu$ we obtain the *time-dependent Bogoliubov-De Gennes equations*:

$$\begin{cases} i\hbar\dfrac{d}{dt}U_{j\mu}(t) = \ \ 2\displaystyle\sum_{j'=1}^{L}\left[A_{jj'}(t)U_{j'\mu}(t) + B_{jj'}(t)V_{j'\mu}(t)\right] \\ i\hbar\dfrac{d}{dt}V_{j\mu}(t) = -2\displaystyle\sum_{j'=1}^{L}\left[B^*_{jj'}(t)U_{j'\mu}(t) + A^*_{jj'}(t)V_{j'\mu}(t)\right] \end{cases} \tag{1.98}$$

or in a more compact way, collecting together $\mu = 1, \cdots, L$ solutions in $L \times L$ blocks $\mathbf{U}$ and $\mathbf{V}$: [18]

$$i\hbar\frac{d}{dt}\begin{pmatrix}\mathbf{U}(t)\\ \mathbf{V}(t)\end{pmatrix} = 2\,\mathbb{H}(t)\cdot\begin{pmatrix}\mathbf{U}(t)\\ \mathbf{V}(t)\end{pmatrix} \ . \tag{1.100}$$

[17] A mathematician would cry, here, that this is not a valid implication: an arbitrary linear combination of $\hat{\gamma}_\mu(t)$ could be added that, acting on $|\psi(t)\rangle$, gives 0. We are a bit swift here, but the result is essentially correct. We will get to the same result by a second quicker route in a short while.

[18] In the time-independent case, the solution is equivalent to solving the time-independent Bogoliubov-De Gennes equations. Indeed in this case the time evolution of the solution is

$$\mathbb{H}\cdot\begin{pmatrix}\mathbf{u}_\mu\\ \mathbf{v}_\mu\end{pmatrix} = \epsilon_\mu\begin{pmatrix}\mathbf{u}_\mu\\ \mathbf{v}_\mu\end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix}\mathbf{u}_\mu(t)\\ \mathbf{v}_\mu(t)\end{pmatrix} = \mathrm{e}^{-2i\epsilon_\mu t/\hbar}\begin{pmatrix}\mathbf{u}_\mu\\ \mathbf{v}_\mu\end{pmatrix} \tag{1.99}$$

and, as you can easily verify, the same result can be obtained by using directly Eq. (1.100) with $\mathbb{H}(t) = \mathbb{H}$.

Notice that if $(\mathbf{u}_\mu(t)\ \mathbf{v}_\mu(t))^T$ is solution of Eq.1.98 then $\left(\mathbf{v}^*_\mu(t)\ \mathbf{u}^*_\mu(t)\right)^T$ is also a solution, so we need to find only $\mu = 1, \cdots, L$ solutions, as indeed alluded by the compact form (1.100), not $2L$. Once we have the first L, it is automatically guaranteed that:

$$i\hbar \frac{d}{dt} \begin{pmatrix} \mathbf{U}(t) & \mathbf{V}^*(t) \\ \mathbf{V}(t) & \mathbf{U}^*(t) \end{pmatrix} = 2\, \mathbb{H}(t) \cdot \begin{pmatrix} \mathbf{U}(t) & \mathbf{V}^*(t) \\ \mathbf{V}(t) & \mathbf{U}^*(t) \end{pmatrix} . \tag{1.101}$$

Second route. It is reassuring to get to the same time-dependent Bogoliubov-de Gennes equations by a second, quicker, route. Let us recall the linear equation we want to solve, with its initial condition:

$$\begin{aligned} i\hbar \frac{d}{dt} \widehat{\mathbf{\Psi}}_H(t) &= 2\, \mathbb{H}(t) \cdot \widehat{\mathbf{\Psi}}_H(t) \\ \widehat{\mathbf{\Psi}}_H(t = t_0) &\equiv \widehat{\mathbf{\Psi}} = \mathbb{U}_0 \cdot \begin{pmatrix} \hat{\boldsymbol{\gamma}} \\ \hat{\boldsymbol{\gamma}}^\dagger \end{pmatrix} \end{aligned}$$

where $\hat{\boldsymbol{\gamma}}$ are the Bogoljubov fermions that diagonalize $\hat{H}(t_0)$, and $\mathbb{U}_0$ the corresponding $2L \times 2L$ rotation matrix. Inspired by the form of the initial condition, let us search for a solution of the same form:

$$\widehat{\mathbf{\Psi}}_H(t) = \mathbb{U}(t) \cdot \begin{pmatrix} \hat{\boldsymbol{\gamma}} \\ \hat{\boldsymbol{\gamma}}^\dagger \end{pmatrix} \tag{1.102}$$

with the *same* $\hat{\boldsymbol{\gamma}}$ used to diagonalize the initial $t = t_0$ problem. In order for this to be a solution, the time-dependent coefficients $\mathbb{U}(t)$ must satisfy the linear Bogoliubov-de Gennes time-dependent equations:

$$i\hbar \frac{d}{dt} \mathbb{U}(t) = 2\mathbb{H}(t) \cdot \mathbb{U}(t) \tag{1.103}$$

with initial conditions $\mathbb{U}(t = t_0) = \mathbb{U}_0$. The latter form is just a compact way of expressing Eq. (1.101).

It is easy to verify that this implies that the operators $\hat{\gamma}_\mu(t)$ in the Schrödinger picture are time-dependent and annihilate the state $|\psi(t)\rangle$: this was indeed the starting point of the Bogoljoubov *Ansatz* presented in the first route. Indeed, since

$$\begin{pmatrix} \hat{\boldsymbol{\gamma}}_H \\ \hat{\boldsymbol{\gamma}}^\dagger_H \end{pmatrix} = \mathbb{U}^\dagger(t) \cdot \begin{pmatrix} \hat{\mathbf{c}}_H(t) \\ \hat{\mathbf{c}}^\dagger_H(t) \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} \hat{\boldsymbol{\gamma}}(t) \\ \hat{\boldsymbol{\gamma}}^\dagger(t) \end{pmatrix} = \mathbb{U}^\dagger(t) \cdot \begin{pmatrix} \hat{\mathbf{c}} \\ \hat{\mathbf{c}}^\dagger \end{pmatrix} \tag{1.104}$$

we can immediately write, in the Schrödinger picture:

$$\hat{\gamma}_\mu(t) = \sum_{j=1}^{L} \left(U^*_{j\mu}(t)\, \hat{c}_j + V^*_{j\mu}(t)\, \hat{c}^\dagger_j \right) . \tag{1.105}$$

If we go back to Sec. 1.5.2, we realize that the algebra carried out there is perfectly applicable here, and allows us to write the time-dependent state $|\psi(t)\rangle$ in the explicit Gaussian form:

$$|\psi(t)\rangle = \mathcal{N}(t)\ \mathrm{e}^{\frac{1}{2}(\hat{\mathbf{c}}^\dagger)^T \cdot \mathbf{Z}(t) \cdot (\hat{\mathbf{c}}^\dagger)}\ |0\rangle = \mathcal{N}(t)\ \exp\left(\frac{1}{2} \sum_{j_1 j_2} Z_{j_1 j_2}(t) \hat{c}^\dagger_{j_1} \hat{c}^\dagger_{j_2} \right) |0\rangle\ , \tag{1.106}$$

with the anti-symmetric matrix $\mathbf{Z}(t)$ given by:

$$\mathbf{Z}(t) = -[\mathbf{U}^\dagger(t)]^{-1} \cdot \mathbf{V}^\dagger(t)\ . \tag{1.107}$$

It is not very hard to explicitly verify that such a state satisfies the Schrödinger equation:

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle \ , \tag{1.108}$$

provided $\mathbf{U}(t)$ and $\mathbf{V}(t)$ satisfy the time-dependent BdG equations in Eq. (1.100). Indeed, the time derivative of the state $|\psi(t)\rangle$ is simply:

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = i\hbar\Big[\frac{1}{2}(\hat{\mathbf{c}}^\dagger)^T\cdot\dot{\mathbf{Z}}(t)\cdot(\hat{\mathbf{c}}^\dagger)+\frac{\dot{\mathcal{N}}(t)}{\mathcal{N}(t)}\Big]|\psi(t)\rangle \ .$$

On the right-hand side, the Hamiltonian terms can be rewritten by using that, for instance:

$$\sum_{jj'}\hat{c}^\dagger_{j'}A_{j'j}\hat{c}_j e^{\mathcal{Z}(t)}|0\rangle = \sum_{jj'}\hat{c}^\dagger_{j'}(\mathbf{A}\cdot\mathbf{Z})_{j'j}\hat{c}^\dagger_j e^{\mathcal{Z}(t)}|0\rangle \ .$$

Rewriting in a similar way all the Hamiltonian terms we get:

$$\hat{H}(t)|\psi(t)\rangle = \Big[(\hat{\mathbf{c}}^\dagger)^T\cdot\Big(\mathbf{B}+\mathbf{A}\cdot\mathbf{Z}+\mathbf{Z}\cdot\mathbf{A}+\mathbf{Z}\cdot\mathbf{B}^*\cdot\mathbf{Z}\Big)\cdot(\hat{\mathbf{c}}^\dagger)-\mathrm{Tr}\mathbf{A}-\mathrm{Tr}\mathbf{B}^*\cdot\mathbf{Z}\Big]|\psi(t)\rangle \ .$$

By explicitly calculating the derivative of $\mathbf{Z}(t)$ using the BdG equations one can check, after some lengthy algebra, that the two expressions indeed coincide. [19]

1.6.2. Calculating time-dependent expectation values.

Once we have a solution of the time-dependent BdG equations, we can calculate time-averages of operators quite easily. Consider, for instance, the elementary one-body Green's function: [20]

$$\begin{aligned} G_{j'j}(t\geq t_0) &\equiv \langle\psi(t)|\hat{c}^\dagger_j\hat{c}_{j'}|\psi(t)\rangle = \langle\psi(t_0)|\hat{c}^\dagger_{jH}(t)\hat{c}_{j'H}(t)|\psi(t_0)\rangle \\ F_{j'j}(t\geq t_0) &\equiv \langle\psi(t)|\hat{c}_j\hat{c}_{j'}|\psi(t)\rangle = \langle\psi(t_0)|\hat{c}_{jH}(t)\hat{c}_{j'H}(t)|\psi(t_0)\rangle \ . \end{aligned} \tag{1.109}$$

We assume that the initial state $|\psi(t_0)\rangle$ is the Bogoljoubov vacuum of the operators $\boldsymbol{\gamma}$ which diagonalize $\hat{H}(t_0)$, i.e., $|\psi(t_0)\rangle = |\emptyset\rangle_\gamma$. Then, simple algebra shows that:

$$\begin{aligned} G_{j'j}(t\geq t_0) &= \Big[\mathbf{V}(t)\cdot\mathbf{V}^\dagger(t)\Big]_{jj'} = \Big[\mathbf{V}^*(t)\cdot\mathbf{V}^T(t)\Big]_{j'j} \stackrel{def}{=} \Big[\mathbf{G}(t)\Big]_{j'j} \\ F_{j'j}(t\geq t_0) &= \Big[\mathbf{U}(t)\cdot\mathbf{V}^\dagger(t)\Big]_{jj'} = \Big[\mathbf{V}^*(t)\cdot\mathbf{U}^T(t)\Big]_{j'j} \stackrel{def}{=} \Big[\mathbf{F}(t)\Big]_{j'j} \ . \end{aligned} \tag{1.110}$$

More generally, you can define the Nambu Green's function

$$\mathbb{G}_{\alpha'\alpha}(t\geq t_0) \equiv \langle\psi(t)|\widehat{\Psi}^\dagger_\alpha\widehat{\Psi}_{\alpha'}|\psi(t)\rangle = \langle\psi(t_0)|\widehat{\Psi}^\dagger_{\alpha H}(t)\widehat{\Psi}_{\alpha' H}(t)|\psi(t_0)\rangle \tag{1.111}$$

and show that the four $L\times L$ blocks of this object read:

$$\mathbb{G}(t\geq t_0) = \left[\begin{array}{c|c} \mathbf{G}(t) & \mathbf{F}^\dagger(t) \\ \hline \mathbf{F}(t) & \mathbf{1}-\mathbf{G}^T(t) \end{array}\right] = \left[\begin{array}{c|c} \mathbf{V}^*(t)\cdot\mathbf{V}^T(t) & \mathbf{U}^*(t)\cdot\mathbf{V}^T(t) \\ \hline \mathbf{V}^*(t)\cdot\mathbf{U}^T(t) & \mathbf{U}^*(t)\cdot\mathbf{U}^T(t) \end{array}\right] \ . \tag{1.112}$$

[19] Indeed, the equation for $\dot{\mathbf{Z}}(t)$ is interesting: it is *non-linear*, and can be written without much difficulty in the case of imaginary-time dynamics as well.

[20] The reason for the definition of the Green's functions with apparently interchanged indices $j'j$, leading to $\mathbf{G}=\mathbf{V}^*\cdot\mathbf{V}^T$ rather then $\mathbf{G}=\mathbf{V}\cdot\mathbf{V}^\dagger$, is that, with this definition, the time-dependent Hartree-Fock equations have a more natural matrix form, see the chapter on time-dependent mean-field methods.

Averages of more complicated operators can be reduced to sums of products of Green's functions through the application of Wick's theorem, which generally applies in the present context. Moreover, time-correlation functions with Heisenberg operators at different times can be calculated in a similar way.

1.6.3. Floquet time-dependent case.

A particular case of dynamics is that in which the Hamiltonian is periodic in time, i.e., a period τ exists such that $\hat{H}(t+\tau) = \hat{H}(t)$. The Floquet theorem (see Chapter on the Floquet dynamics) guarantees the existence in the Hilbert space of a complete basis of solutions of the time-dependent Schrödinger equation which are *periodic "up to a phase factor"*, i.e., such that:

$$|\psi_{F\alpha}(t)\rangle = \mathrm{e}^{-i\overline{\mu}_\alpha t/\hbar}\,|\psi_{P\alpha}(t)\rangle \qquad \text{with} \qquad |\psi_{P\alpha}(t)\rangle = |\psi_{P\alpha}(t+\tau)\rangle \ .$$

This way of writing is closely reminiscent of the time-independent case, except that the state $|\psi_{P\alpha}(t)\rangle$, known as *Floquet mode*, is now *periodic* in time rather then a time-independent eigenstate of the Hamiltonian; the $\overline{\mu}_\alpha$, which plays the role of the eigenenergy, is known as *Floquet quasi-energy*. There are 2^L, as many as the dimension of the Hilbert space, Floquet solutions of this type, and these solutions can be used as a convenient time-dependent basis to expand states. Their usefulness consist in the fact that if we expand a general initial state as $|\psi(0)\rangle = \sum_\alpha |\psi_{P\alpha}(0)\rangle\langle\psi_{P\alpha}(0)|\psi(0)\rangle$, then the time-evolution can be written, for free, in a form that is reminiscent of the time-independent case, i.e.:

$$|\psi(t)\rangle = \underbrace{\sum_{\alpha=1}^{2^L} \mathrm{e}^{-i\overline{\mu}_\alpha t/\hbar}\ |\psi_{P\alpha}(t)\rangle\,\langle\psi_{P\alpha}(0)}_{\hat{U}(t)}\,|\psi(0)\rangle \ . \tag{1.113}$$

An explicit construction of the many-body Floquet states can be obtained through a Floquet analysis of the time-dependent Bogoliubov-de Gennes equations, in a way similar to that used to construct the energy eigenstates from the solution of the static Bogoliubov-de Gennes equations (see Sec. 1.5). To do that, let us write the Bogoliubov-de Gennes equations (1.115)

$$i\hbar\frac{d}{dt}\begin{pmatrix}\mathbf{U}(t)\\ \mathbf{V}(t)\end{pmatrix} = 2\mathbb{H}(t)\cdot\begin{pmatrix}\mathbf{U}(t)\\ \mathbf{V}(t)\end{pmatrix} \ . \tag{1.114}$$

Since $\mathbb{H}(t+\tau) = \mathbb{H}(t)$ is a periodic $2L\times 2L$ matrix, the Floquet theorem guarantees the existence of a complete set of $2L$ solutions which are periodic up to a phase. L of them have the form:

$$\mathrm{e}^{-i\mu_\alpha t/\hbar}\begin{pmatrix}\mathbf{u}_{P\alpha}(t)\\ \mathbf{v}_{P\alpha}(t)\end{pmatrix} \qquad \text{for } \alpha = 1\cdots L \qquad \text{with} \begin{cases}\mathbf{u}_{P\alpha}(t+\tau) = \mathbf{u}_{P\alpha}(t)\\ \mathbf{v}_{P\alpha}(t+\tau) = \mathbf{v}_{P\alpha}(t)\end{cases},$$

and the remaining L, by particle-hole symmetry, are automatically obtained as $\mathrm{e}^{i\mu_\alpha t}\,(\mathbf{v}^*_{P\alpha}(t)\ \mathbf{u}^*_{P\alpha}(t))^T$. Collecting all the quasi-energies μ_α into a diagonal matrix $\boldsymbol{\mu} = \mathrm{diag}(\mu_\alpha)$, and the various column vectors $\mathbf{u}_{P\alpha}(t)$ and $\mathbf{v}_{P\alpha}(t)$ into a $L\times L$ matrices $\mathbf{U}_P(t)$ and $\mathbf{V}_P(t)$, it is straitghforward

to show that the structure of the Floquet solutions of the Bogoliubov-de Gennes solutions is [21]

$$\mathbb{U}_F(t) = \left(\begin{array}{c|c} \mathbf{U}_F(t) & \mathbf{V}_F^*(t) \\ \hline \mathbf{V}_F(t) & \mathbf{U}_F^*(t) \end{array}\right) = \left(\begin{array}{c|c} \mathbf{U}_P(t)\cdot e^{-i\boldsymbol{\mu}t/\hbar} & \mathbf{V}_P^*(t)\cdot e^{i\boldsymbol{\mu}t/\hbar} \\ \hline \mathbf{V}_P(t)\cdot e^{-i\boldsymbol{\mu}t/\hbar} & \mathbf{U}_P^*(t)\cdot e^{i\boldsymbol{\mu}t/\hbar} \end{array}\right) \tag{1.115}$$

Using these solutions, we can construct the Bogoliubov operators $\hat{\gamma}_{F\alpha}(t)$ which annihilate a vacuum Floquet state $|\emptyset_F(t)\rangle$ through the standard method employed in the general time-dependent case (see Eq. 1.59):

$$\begin{pmatrix} \hat{\boldsymbol{\gamma}}_F(t) \\ \hat{\boldsymbol{\gamma}}_F^\dagger(t) \end{pmatrix} = \mathbb{U}_F^\dagger(t)\cdot \begin{pmatrix} \hat{\mathbf{c}} \\ \hat{\mathbf{c}}^\dagger \end{pmatrix} \tag{1.116}$$

or, more explicitly, for $\alpha = 1, \cdots, L$:

$$\hat{\gamma}_{F\alpha}(t) = \mathrm{e}^{i\mu_\alpha t}\sum_{j=1}^{L}\left(U^*_{Pj\alpha}(t)\hat{c}_j + V^*_{Pj\alpha}(t)\hat{c}_j^\dagger\right) \quad \Rightarrow \quad \hat{\gamma}_{F\alpha}(t+\tau) = \mathrm{e}^{i\mu_\alpha\tau}\hat{\gamma}_{F\alpha}(t) \quad \forall t\,. \tag{1.117}$$

The Floquet vacuum state $|\emptyset_F(t)\rangle$ annihilated by all the $\hat{\gamma}_{F\alpha}(t)$ has the Gaussian form (see Eq. (1.106)):

$$|\emptyset_F(t)\rangle = \mathcal{N}_F(t)\; e^{\frac{1}{2}(\hat{\mathbf{c}}^\dagger)^T\cdot\mathbf{Z}_F(t)\cdot(\hat{\mathbf{c}}^\dagger)}\;|0\rangle \tag{1.118}$$

where, see Secs. 1.5 and 1.6, the Thouless and Onishi formulas hold:

$$\mathbf{Z}_F(t) = -[\mathbf{U}_F^\dagger(t)]^{-1}\cdot\mathbf{V}_F^\dagger(t) \qquad \text{and} \qquad \mathcal{N}_F(t) = \sqrt{|\det[\mathbf{U}_F(t)]|}\,. \tag{1.119}$$

Let us show that the Floquet vacuum state is periodic, i.e.,

$$|\emptyset_F(t+\tau)\rangle = |\emptyset_F(t)\rangle\,,$$

or, to put it differently, its many-body quasi-energy is $\overline{\mu}_0 = 0$. To this aim it suffices to show that $\mathbf{Z}_F(t)$ and $\mathcal{N}_F(t)$ are both periodic. From $\mathbf{V}_F = \mathbf{V}_P\cdot e^{-i\boldsymbol{\mu}t/\hbar}$ and $\mathbf{U}_F = \mathbf{U}_P\cdot e^{-i\boldsymbol{\mu}t/\hbar}$ we immediately derive that $\mathbf{V}_F^\dagger(t) = e^{i\boldsymbol{\mu}t/\hbar}\cdot\mathbf{V}_P^\dagger(t)$ and $[\mathbf{U}_F^\dagger(t)]^{-1} = [\mathbf{U}_P^\dagger(t)]^{-1}\cdot e^{-i\boldsymbol{\mu}t/\hbar}$. From these relationships, in turn, it follows immediately that the quasi-energy phase-factors cancel in $\mathbf{Z}_F$, i.e.:

$$\mathbf{Z}_F(t) = -[\mathbf{U}_F^\dagger(t)]^{-1}\cdot\mathbf{V}_F^\dagger(t) = -[\mathbf{U}_P^\dagger(t)]^{-1}\cdot\mathbf{V}_P^\dagger(t)\,, \tag{1.120}$$

which is manifestly periodic in time, $\mathbf{Z}_F(t+\tau) = \mathbf{Z}_F(t)$, because both $\mathbf{U}_P$ and $\mathbf{V}_P$ are periodic. The periodicity of $\mathcal{N}_F(t)$ follows because

$$|\det[\mathbf{U}_F(t)]| = |\det[\mathbf{U}_P(t)]\,\det[e^{-i\boldsymbol{\mu}t/\hbar}]| = |\det[\mathbf{U}_P(t)]||e^{-i\sum_\alpha\mu_\alpha t/\hbar}| = |\det[\mathbf{U}_P(t)]|\,,$$

i.e., once again something manifestly periodic in time. At this point, we can easily, in principle, construct all the 2^L many-body Floquet states by simply applying any product of $\hat{\gamma}_{F\alpha}^\dagger(t)$ to $|\emptyset_F(t)\rangle$: [22]

$$|\psi_{F\{n_\alpha\}}(t)\rangle = \prod_{\alpha=1}^{L}[\hat{\gamma}_{F\alpha}^\dagger(t)]^{n_\alpha}|\emptyset_F(t)\rangle\,, \tag{1.121}$$

[21] Notice that the quasi-energy phase factors have to stay on the *right* of the periodic part, in order for the ordinary rules of matrix multiplication to give the correct phase-factor to each *column* of the matrix.

[22] Some care should be exercised if the boundary conditions depend on the fermionic parity. In that case, one should work separately in the two subsectors with even and odd fermionic parity, starting from the corresponding vacuum state.

where $n_\alpha = 0$ or 1 is the occupation number of the $\hat{\gamma}^\dagger_{F\alpha}(t)$ operator. From Eq. (1.117) and the periodicity of the Floquet vacuum, it follows that the quasi-energy of $|\psi_{F\{n_\alpha\}}(t)\rangle$ is given by:

$$\overline{\mu}_{\{n_\alpha\}} = \sum_{\alpha=1}^{L} n_\alpha \mu_\alpha \ . \tag{1.122}$$

1.7. Overlap between BCS states in Ising/XY chains

Sometimes, for instance in the context of quantum quenches, where the Hamiltonian is abruptly changed, it is important to know how to calculate the overlap between BCS states belonging to two different Ising Hamiltonians $\hat{H}_0$ and $\hat{H}_1$. Let us start considering the two BCS ground states of $\hat{H}_0$ and $\hat{H}_1$. These two states are Bogoljoubov vacua with respect to the fermionic operators $\hat{\gamma}_{0\mu}$ and $\hat{\gamma}_{1\mu}$, and we donote them, for a more compact notation, as $|\emptyset\rangle_{\gamma_0} = |\emptyset_0\rangle$ and $|\emptyset\rangle_{\gamma_1} = |\emptyset_1\rangle$ We will first compute $|\langle\emptyset_1\,|\emptyset_0\rangle\,|^2$, and then we will extend the result to the overlap of general excited states. The two sets of fermions can be written in terms of the original Jordan-Wigner fermions as:

$$\begin{pmatrix} \hat{\boldsymbol{\gamma}}_{0(1)} \\ \hat{\boldsymbol{\gamma}}^\dagger_{0(1)} \end{pmatrix} = \mathbb{U}^\dagger_{0(1)} \cdot \hat{\boldsymbol{\Psi}} = \begin{pmatrix} \mathbf{U}^\dagger_{0(1)} & \mathbf{V}^\dagger_{0(1)} \\ \mathbf{V}^T_{0(1)} & \mathbf{U}^T_{0(1)} \end{pmatrix} \cdot \begin{pmatrix} \hat{\mathbf{c}} \\ \hat{\mathbf{c}}^\dagger \end{pmatrix} . \tag{1.123}$$

We can write the direct unitary transformation from one set to the other as follow:

$$\begin{pmatrix} \hat{\boldsymbol{\gamma}}_1 \\ \hat{\boldsymbol{\gamma}}^\dagger_1 \end{pmatrix} = \mathbb{U}^\dagger_1 \cdot \mathbb{U}_0 \cdot \begin{pmatrix} \hat{\boldsymbol{\gamma}}_0 \\ \hat{\boldsymbol{\gamma}}^\dagger_0 \end{pmatrix} = \mathbb{U}^\dagger \cdot \begin{pmatrix} \hat{\boldsymbol{\gamma}}_0 \\ \hat{\boldsymbol{\gamma}}^\dagger_0 \end{pmatrix} = \begin{pmatrix} \mathbf{U}^\dagger & \mathbf{V}^\dagger \\ \mathbf{V}^T & \mathbf{U}^T \end{pmatrix} \cdot \begin{pmatrix} \hat{\boldsymbol{\gamma}}_0 \\ \hat{\boldsymbol{\gamma}}^\dagger_0 \end{pmatrix} , \tag{1.124}$$

where:

$$\mathbb{U} \equiv \begin{pmatrix} \mathbf{U} & \mathbf{V}^* \\ \mathbf{V} & \mathbf{U}^* \end{pmatrix} , \tag{1.125}$$

with:

$$\mathbf{U} = \mathbf{U}^\dagger_0 \cdot \mathbf{U}_1 + \mathbf{V}^\dagger_0 \cdot \mathbf{V}_1 \qquad\qquad \mathbf{V} = \mathbf{V}^T_0 \cdot \mathbf{U}_1 + \mathbf{U}^T_0 \cdot \mathbf{V}_1 \ . \tag{1.126}$$

We will prove that, if $|\emptyset_0\rangle$ and $|\emptyset_1\rangle$ are not orthogonal, then:

$$|\langle\emptyset_1|\emptyset_0\rangle|^2 = |\det[\mathbf{U}]| \ , \tag{1.127}$$

a relationship which is known as *Onishi formula*. Indeed, we have already given a proof of this relationship in Sec. 1.5.2, for the special case in which one of the two sets of fermions where the original Jordan-Wigner fermions $\hat{c}_j$ with associated vacuum state $|0\rangle$. There we showed that, with the present notation:

$$|\emptyset_{0(1)}\rangle = \mathcal{N}_{0(1)}\ e^{\frac{1}{2}(\hat{\mathbf{c}}^\dagger)^T \cdot \mathbf{Z}_{0(1)} \cdot (\hat{\mathbf{c}}^\dagger)}\ |0\rangle \tag{1.128}$$

with:

$$\mathbf{Z}_{0(1)} = -[\mathbf{U}^\dagger_{0(1)}]^{-1} \cdot \mathbf{V}^\dagger_{0(1)} \ , \tag{1.129}$$

and $|\langle 0|\emptyset_{0(1)}\rangle|^2 = |\mathcal{N}_{0(1)}|^2 = |\det[\mathbf{U}_{0(1)}]|$. With exactly the same algebra, we could establish, for instance, that:

$$|\emptyset_1\rangle = \mathcal{N}\ e^{\hat{\mathcal{Z}}}|\emptyset_0\rangle = \mathcal{N}\ e^{\frac{1}{2}(\hat{\boldsymbol{\gamma}}^\dagger_0)^T \cdot \mathbf{Z} \cdot (\hat{\boldsymbol{\gamma}}^\dagger_0)}\ |\emptyset_0\rangle \ , \tag{1.130}$$

with:

$$\mathbf{Z} = -[\mathbf{U}^\dagger]^{-1} \cdot \mathbf{V}^\dagger \,, \tag{1.131}$$

and $|\langle \emptyset_0 | \emptyset_1 \rangle|^2 = |\mathcal{N}|^2 = |\det[\mathbf{U}]|$. But there are a number of points where we were a bit swift, in this derivation: for instance, we assumed that $\mathbf{U}$ is invertible, which is not guaranteed. The issue about a possible orthogonality was also not raised. Moreover, the case in which the resulting ground state is a pure Slater determinant *without BCS-pairing*, a case which is relevant for the XY model, is not clearly discussed in this way.

We will now give an alternative proof which makes use of an interesting theorem due to Bloch and Messiah [2], and which clarifies all these issues. We will perform an intermediate canonical transformation which first allows us to write an explicit equation for $|\emptyset_1\rangle$ in terms of $|\emptyset_0\rangle$, and then to compute easily $\langle \emptyset_1 | \, \emptyset_0 \rangle$. The theorem that Bloch and Messiah proved [2] shows that matrices with the structure of $\mathbb{U}$ above can be decomposed into a product of three unitary transformations as follows:

$$\mathbb{U} = \begin{pmatrix} \mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{D}^* \end{pmatrix} \begin{pmatrix} \overline{\mathbf{U}} & \overline{\mathbf{V}} \\ \overline{\mathbf{V}} & \overline{\mathbf{U}} \end{pmatrix} \begin{pmatrix} \mathbf{C} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}^* \end{pmatrix} \,, \tag{1.132}$$

where $\mathbf{D}$, $\mathbf{C}$ are $L \times L$ unitary matrices and $\overline{\mathbf{U}}$, $\overline{\mathbf{V}}$ are $L \times L$ real matrices of the form:

$$\overline{\mathbf{U}} = \begin{pmatrix} 0 & & & & & & & & & \\ & \ddots & & & & & & & & \\ & & 0 & & & & & & & \\ & & & u_1 & 0 & & & & & \\ & & & 0 & u_1 & & & & & \\ & & & & & \ddots & & & & \\ & & & & & & u_n & 0 & & \\ & & & & & & 0 & u_n & & \\ & & & & & & & & 1 & \\ & & & & & & & & & \ddots \\ & & & & & & & & & 1 \end{pmatrix}$$

$$\overline{\mathbf{V}} = \begin{pmatrix} 1 & & & & & & & & & \\ & \ddots & & & & & & & & \\ & & 1 & & & & & & & \\ & & & 0 & v_1 & & & & & \\ & & & -v_1 & 0 & & & & & \\ & & & & & \ddots & & & & \\ & & & & & & 0 & v_n & & \\ & & & & & & -v_n & 0 & & \\ & & & & & & & & 0 & \\ & & & & & & & & & \ddots \\ & & & & & & & & & 0 \end{pmatrix} \tag{1.133}$$

in which $u_p > 0$, $v_p > 0$ and $u_p^2 + v_p^2 = 1$. From these relations we have:

$$\mathbf{U} = \mathbf{D} \cdot \overline{\mathbf{U}} \cdot \mathbf{C} \qquad\qquad \mathbf{V} = \mathbf{D}^* \cdot \overline{\mathbf{V}} \cdot \mathbf{C} \,. \tag{1.134}$$

The idea is the following. Since:

$$\begin{pmatrix} \hat{\gamma}_0 \\ \hat{\gamma}_0^\dagger \end{pmatrix} = \mathbb{U} \cdot \begin{pmatrix} \hat{\gamma}_1 \\ \hat{\gamma}_1^\dagger \end{pmatrix} = \begin{pmatrix} \mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{D}^* \end{pmatrix} \begin{pmatrix} \overline{\mathbf{U}} & \overline{\mathbf{V}} \\ \overline{\mathbf{V}} & \overline{\mathbf{U}} \end{pmatrix} \begin{pmatrix} \mathbf{C} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}^* \end{pmatrix} \begin{pmatrix} \hat{\gamma}_1 \\ \hat{\gamma}_1^\dagger \end{pmatrix} \tag{1.135}$$

we can think of the transformation as the product of: (1) a first unitary transformation $\mathbf{C}$ which does not mix particles and holes for fermions $\hat{\boldsymbol{\gamma}}_1$, defined by

$$\begin{pmatrix} \hat{\boldsymbol{\alpha}}_1 \\ \hat{\boldsymbol{\alpha}}_1^\dagger \end{pmatrix} = \begin{pmatrix} \mathbf{C} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}^* \end{pmatrix} \cdot \begin{pmatrix} \hat{\gamma}_1 \\ \hat{\gamma}_1^\dagger \end{pmatrix} \tag{1.136}$$

followed by (2) a simple "canonical form" of a transformation leading to new fermions:

$$\begin{pmatrix} \hat{\boldsymbol{\alpha}}_0 \\ \hat{\boldsymbol{\alpha}}_0^\dagger \end{pmatrix} = \begin{pmatrix} \overline{\mathbf{U}} & \overline{\mathbf{V}} \\ \overline{\mathbf{V}} & \overline{\mathbf{U}} \end{pmatrix} \cdot \begin{pmatrix} \hat{\boldsymbol{\alpha}}_1 \\ \hat{\boldsymbol{\alpha}}_1^\dagger \end{pmatrix} . \tag{1.137}$$

The final transformation (3) leading to the fermions $\hat{\boldsymbol{\gamma}}_0$ is again a unitary $\mathbf{D}$ which does not mix particles and holes:

$$\begin{pmatrix} \hat{\boldsymbol{\gamma}}_0 \\ \hat{\boldsymbol{\gamma}}_0^\dagger \end{pmatrix} = \begin{pmatrix} \mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{D}^* \end{pmatrix} \cdot \begin{pmatrix} \hat{\boldsymbol{\alpha}}_0 \\ \hat{\boldsymbol{\alpha}}_0^\dagger \end{pmatrix} . \tag{1.138}$$

In essence, what the theorem guarantees is that one can always find a basis such that the transformed fermions, $\hat{\boldsymbol{\alpha}}_0$ and $\hat{\boldsymbol{\alpha}}_1$, are coupled by a particularly simple matrix in which there are only three possibilities: *(i)* for some indices, which we denote by l, there is no transformation at all (the ones in the diagonal of $\overline{\mathbf{U}}$), i.e., $\hat{\alpha}_{1l} = \hat{\alpha}_{0l}$; *(ii)* for some other indices, which we donote by k, the transformation is a pure particle-hole $\hat{\alpha}_{1k}^\dagger = \hat{\alpha}_{0k}$: these indices correspond to the zeroes in the diagonal of $\overline{\mathbf{U}}$, and the ones in the diagonal of $\overline{\mathbf{V}}$; *(iii)* all other indices, denoted by $(p, \overline{p})$, are BCS-paired in a simple way, and they form 2×2 blocks in the matrices $\overline{\mathbf{U}}$ and $\overline{V}$ with coefficients u_p and v_p, such that:

$$\begin{aligned} \hat{\alpha}_{1p}^\dagger &= u_p \hat{\alpha}_{0p}^\dagger - v_p \hat{\alpha}_{0\overline{p}} \\ \hat{\alpha}_{1\overline{p}}^\dagger &= u_p \hat{\alpha}_{0\overline{p}}^\dagger + v_p \hat{\alpha}_{0p} . \end{aligned} \tag{1.139}$$

We must stress that the theorem does not tell us *how many* indices belong to the three cathegories above: in some cases all the indices might be 2×2-paired, but it is also possible that the transformation is a pure particle-hole transoformation without any pairing at all.

The construction of the relationship between $|\emptyset_0\rangle$ and $|\emptyset_1\rangle$ becomes particularly simple in terms for the fermions $\hat{\boldsymbol{\alpha}}_{0(1)}$. The key idea is the $\hat{\boldsymbol{\alpha}}_{0(1)}$ is related to $\hat{\boldsymbol{\gamma}}_{0(1)}$ by a transformation which does not mix particles and holes, and therefore it is still true that $\hat{\alpha}_{0n} |\emptyset_0\rangle = 0$ and $\hat{\alpha}_{1n} |\emptyset_1\rangle = 0$. Since $|\emptyset_1\rangle$ is the state which is annihilated by any $\hat{\alpha}_{1n}$ we can write it as:

$$|\emptyset_1\rangle = \mathcal{N} \prod_n \hat{\alpha}_{1n} |\emptyset_0\rangle = \prod_k \hat{\alpha}_{0k}^\dagger \prod_p \left(u_p + v_p \hat{\alpha}_{0p}^\dagger \hat{\alpha}_{0\overline{p}}^\dagger \right) |\emptyset_0\rangle \ , \tag{1.140}$$

where $\mathcal{N}$ is a normalization constant. Notice that we included only BCS-paired indices and particle-hole transformed k-indices but *not* l-indices, since $\hat{\alpha}_{1l} = \hat{\alpha}_{0l}$ and the inclusion of such terms would give zero, since $\hat{\alpha}_{0l} |\emptyset_0\rangle = 0$. Since, by hypothesis, the two states $|\emptyset_0\rangle$ and $|\emptyset_1\rangle$ are not orthogonal there should not be pure particles-holes k-indices either, and therefore:

$$\langle \emptyset_0 | \emptyset_1 \rangle = \langle \emptyset_0 | \prod_p \left(u_p + v_p \hat{\alpha}_{0p}^\dagger \hat{\alpha}_{0\overline{p}}^\dagger \right) |\emptyset_0\rangle = \prod_p u_p = \sqrt{\prod_p u_p^2} = \sqrt{\det[\overline{\mathbf{U}}]} . \tag{1.141}$$

Finally, since $\overline{\mathbf{U}} = \mathbf{D}^\dagger \cdot \mathbf{U} \cdot \mathbf{C}^\dagger$, and $\mathbf{D}$, and $\mathbf{C}$ are unitary transformations:

$$|\langle \emptyset_0 \, | \emptyset_1 \rangle \, |^2 = |\det[\mathbf{D}^\dagger \cdot \mathbf{U} \cdot \mathbf{C}^\dagger]| = |\det[\mathbf{U}]| \, , \tag{1.142}$$

which is what we wanted to show.

The extension to the calculation of the overlap between $|\emptyset_0\rangle$ and any eigenstate $|\{n_{1\mu}\}\rangle = \prod_{\mu \in I} \hat{\gamma}^\dagger_{1\mu} |\emptyset_1\rangle$, where I is the set of occupied states ($n_{1\mu} = 1$), is in principle straightforward. Here is a possible way to tackle the problem. This state can be thought as an empty set with respect to the following new set of fermions:

$$\hat{\beta}^\dagger_\mu = \hat{\gamma}^\dagger_{1\mu} \quad \text{if } \mu \notin I \qquad\qquad \hat{\beta}^\dagger_\mu = \hat{\gamma}_{1\mu} \quad \text{if } \mu \in I \, , \tag{1.143}$$

in which we have performed a particle-hole transformation for the occupied modes. Now we can use the equation obtained for the scalar product between empty states, i.e.,

$$|\langle \emptyset_0 | \, \{n_{1\mu}\} \rangle|^2 = \left|\det[\mathbf{U}']\right| \, , \tag{1.144}$$

where the matrix $\mathbf{U}'$ is:

$$\mathbf{U}' = \mathbf{U}_0^\dagger \cdot \mathbf{U}_1' + \mathbf{V}_0^\dagger \cdot \mathbf{V}_1' \, , \tag{1.145}$$

in which:

$$\begin{aligned} U'_{1j\mu} &= U_{1j\mu} \quad \text{if } \mu \notin I \qquad & U'_{1j\mu} &= V^*_{1j\mu} \quad \text{if } \mu \in I \\ V'_{1j\mu} &= V_{1j\mu} \quad \text{if } \mu \notin I \qquad & V'_{1j\mu} &= U^*_{1j\mu} \quad \text{if } \mu \in I \, . \end{aligned} \tag{1.146}$$

A second approach to calculate these overlaps with excited states makes explicit use of the Gaussian nature of the states. The relevant algebra follows directly from that of Sec. 1.5.2. Let us start by considering the overlap bewteen $\hat{\gamma}^\dagger_{0\mu_1} \hat{\gamma}^\dagger_{0\mu_2} |\emptyset_0\rangle$ and $|\emptyset_1\rangle = \mathcal{N} e^{\mathcal{Z}} |\emptyset_0\rangle$. This is given by:

$$\begin{aligned} \langle \emptyset_0 | \hat{\gamma}_{0\mu_2} \hat{\gamma}_{0\mu_1} | \emptyset_1 \rangle &= \mathcal{N} \langle \emptyset_0 | \hat{\gamma}_{0\mu_2} \hat{\gamma}_{0\mu_1} e^{\mathcal{Z}} | \emptyset_0 \rangle \\ &= \mathcal{N} \langle \emptyset_0 | e^{\mathcal{Z}} \Big(\hat{\gamma}_{0\mu_2} + \sum_{\mu'_2} Z_{\mu_2 \mu'_2} \hat{\gamma}^\dagger_{0\mu'_2} \Big) \Big(\hat{\gamma}_{0\mu_1} + \sum_{\mu'_1} Z_{\mu_1 \mu'_1} \hat{\gamma}^\dagger_{0\mu'_1} \Big) | \emptyset_0 \rangle \\ &= \mathcal{N} \langle \emptyset_0 | e^{\mathcal{Z}} \hat{\gamma}_{0\mu_2} \Big(\sum_{\mu'_1} Z_{\mu_1 \mu'_1} \hat{\gamma}^\dagger_{0\mu'_1} \Big) | \emptyset_0 \rangle = \langle \emptyset_0 | \emptyset_1 \rangle \; Z_{\mu_1 \mu_2} \, , \end{aligned}$$

where in the second step we have made use of the commutation property:

$$\hat{\gamma}_{0\mu} e^{\mathcal{Z}} = e^{\mathcal{Z}} \left(\hat{\gamma}_{0\mu} + [\hat{\gamma}_{0\mu}, \mathcal{Z}] \right) = e^{\mathcal{Z}} \left(\hat{\gamma}_{0\mu} + \sum_{\mu'} Z_{\mu\mu'} \hat{\gamma}^\dagger_{0\mu'} \right) . \tag{1.147}$$

Notice that, in order for the overlap to be non-vanishing, we were forced to contract $\hat{\gamma}_{0\mu_2}$ against $\hat{\gamma}^\dagger_{0\mu'_1}$ in the final step. A similar calculation shows that, if we have an *even* number $2n$ of operator, the result is highly reminiscent of a Wick's theorem sum-of-products of contractions:

$$\begin{aligned} \langle \emptyset_0 | \hat{\gamma}_{0\mu_{2n}} \cdots \hat{\gamma}_{0\mu_1} | \emptyset_1 \rangle &= \mathcal{N} \langle \emptyset_0 | e^{\mathcal{Z}} \Big(\hat{\gamma}_{0\mu_{2n}} + \sum_{\mu'_{2n}} Z_{\mu_{2n}\mu'_{2n}} \hat{\gamma}^\dagger_{0\mu'_{2n}} \Big) \cdots \Big(\hat{\gamma}_{0\mu_1} + \sum_{\mu'_1} Z_{\mu_1 \mu'_1} \hat{\gamma}^\dagger_{0\mu'_1} \Big) | \emptyset_0 \rangle \\ &= \langle \emptyset_0 | \emptyset_1 \rangle \sum_P (-1)^P Z_{\mu_{P_1}\mu_{P_2}} Z_{\mu_{P_3}\mu_{P_4}} \cdots Z_{\mu_{P_{2n-1}}\mu_{P_{2n}}} \\ &= \langle \emptyset_0 | \emptyset_1 \rangle \; \mathrm{Pf} \, [\mathbf{Z}]_{2n \times 2n} \, , \end{aligned} \tag{1.148}$$

while the overlap vanishes for an odd number of $\hat{\gamma}_{o\mu_i}$. In the last expression, the Wick's sum is rewritten in terms of the so-called *Pfaffian* of the anti-symmetric matrix $\mathbf{Z}$ (or more properly, of the $2n \times 2n$ elements of $\mathbf{Z}$ required by the indices $\mu_1 \cdots \mu_{2n}$):

$$\begin{aligned} \mathrm{Pf}\,[\mathbf{Z}]_{2n\times 2n} &= \mathrm{Pf}\begin{bmatrix} 0 & Z_{\mu_1\mu_2} & Z_{\mu_1\mu_3} & \cdots & Z_{\mu_1\mu_{2n}} \\ Z_{\mu_2\mu_1} & 0 & Z_{\mu_2\mu_3} & \cdots & Z_{\mu_2\mu_{2n}} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ Z_{\mu_{2n}\mu_1} & Z_{\mu_{2n}\mu_2} & Z_{\mu_{2n}\mu_3} & \cdots & 0 \end{bmatrix} \\ &\stackrel{def}{=} \sum_P (-1)^P \underbrace{Z_{\mu_{P_1}\mu_{P_2}} Z_{\mu_{P_3}\mu_{P_4}} \cdots Z_{\mu_{P_{2n-1}}\mu_{P_{2n}}}}_{n \text{ factors}} . \end{aligned} \tag{1.149}$$

Notice that the Pfaffian is really defined by a Wick's sum which contains n products of $\mathbf{Z}$-matrix elements, and not $2n$, as the familiar $\det[\mathbf{Z}]_{2n\times 2n}$. However, a remarkable identity exists (see the book by McCoy) which links the two objects:

$$\begin{aligned} \det[\mathbf{Z}]_{2n\times 2n} &= \sum_P (-1)^P \underbrace{Z_{\mu_1\mu_{P_1}} Z_{\mu_2\mu_{P_2}} \cdots Z_{\mu_{2n}\mu_{P_{2n}}}}_{2n \text{ factors}} \\ &= \left(\mathrm{Pf}\,[\mathbf{Z}]_{2n\times 2n}\right)^2 . \end{aligned} \tag{1.150}$$

Notice, however, that the link exsists only if the dimension of the antisymmetric matrix we are considering is *even*: The determinant of an odd-dimension anti-symmetric matrix is simply zero, while the Pfaffian is not defined. Summarizing, we have obtained the generalization of the Onishi formula in the form:

$$\langle \emptyset_0 | \hat{\gamma}_{0\mu_{2n}} \cdots \hat{\gamma}_{0\mu_1} | \emptyset_1 \rangle = \langle \emptyset_0 | \emptyset_1 \rangle \ \mathrm{Pf}\,[\mathbf{Z}]_{2n\times 2n} = \langle \emptyset_0 | \emptyset_1 \rangle \ \left(\det[\mathbf{Z}]_{2n\times 2n}\right)^{1/2} . \tag{1.151}$$

1.8. The special case of Slater determinants

The approach so far has treated on an equal footing generalized-BCS states and Slater determinants, but the latter are clearly a very special case of the former, when no pairing exists. We devote this paragraph to showing how this special case, of great relavant to many problems including XY chains, can be dealt with in a way which is computationally less intensive (albeit formally less appealing, because of the lack of an explicit particle-hole symmetry). The Bloch-Messiah theorem clearly applies even when no pairing is present, but the form of the matrices $\overline{\mathbf{U}}$ and $\overline{\mathbf{V}}$ is particularly simple:

$$\overline{\mathbf{U}} = \left(\begin{array}{c|c} \mathbf{0}_{N_p} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{1}_{L-N_p} \end{array}\right) \qquad \text{and} \qquad \overline{\mathbf{V}} = \left(\begin{array}{c|c} \mathbf{1}_{N_p} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0}_{L-N_p} \end{array}\right) , \tag{1.152}$$

where $N_h + N_p = L$. This in turn implies, using Eq. (1.137), that:

$$\begin{aligned} \hat{\alpha}_{0k} &= \hat{\alpha}^\dagger_{1k} \qquad \text{for } k = 1, \cdots, N_p \\ \hat{\alpha}_{0l} &= \hat{\alpha}_{1l} \qquad \text{for } l = N_p + 1, \cdots, L . \end{aligned}$$

In words, there are N_p occupied states, meaning that if $|0\rangle = |\emptyset_1\rangle$ is the vacuum state of the fermions $\hat{\alpha}_{1n}$, then a properly defined vacuum state for the fermions $\hat{\alpha}_{1n}$ is just the Slater

determinant:

$$|\emptyset_0\rangle = \prod_{k=1}^{N_p} \hat{\alpha}^\dagger_{1k}|0\rangle \qquad \Rightarrow \qquad \hat{\alpha}_{0n}|\emptyset_0\rangle = 0 \quad \forall n \ . \tag{1.153}$$

Transformations of this type are called *particle-hole* transformations. We see very clearly that $\overline{\mathbf{U}}$ cannot be inverted, because of the N_p zeroes in the diagonal.

Now suppose $|\emptyset_0\rangle$ and $|\emptyset_1\rangle$ are both Slater determinants which are the ground state of two quadratic Hamiltonians $\hat{H}_0$ and $\hat{H}_1$ without anomalous BCS-like terms. We then ask: how do we write a Thouless formula relating these two Slater determinant states? [23] The answer is a special case of the general expression. If $|\emptyset_0\rangle = \prod_{k=1}^{N_p} \hat{a}^\dagger_k|0\rangle$, where we have denoted $\hat{\alpha}_{1k} = \hat{a}_k$, then:

$$|\emptyset_1\rangle = \mathcal{N} \prod_{k=1}^{N_p} \prod_{l=N_p+1}^{L} \left(1 + Z_{kl}\hat{a}^\dagger_l \hat{a}_k\right)|\emptyset_0\rangle = \mathcal{N} \exp\left(\sum_{k=1}^{N_p}\sum_{l=N_p+1}^{L} Z_{kl}\hat{a}^\dagger_l\hat{a}_k\right)|\emptyset_0\rangle \ . \tag{1.154}$$

Notice that there is no requirement on Z_{kl} being antisymmetric in the present context, since by definition k are the N_p occupied indices in the Slater determinant $|\emptyset_0\rangle$ while l runs over all the remaining unoccupied indices.

Let us see how this can be rederived by assuming, from the start, the absence of BCS terms. We will hence the Hamiltonian to be of the general quadratic form:

$$\hat{H}(t) = \sum_{j'j} h_{j'j}(t)\ \hat{c}^\dagger_{j'}\hat{c}_j \ , \tag{1.155}$$

where $h_{j'j} = h^*_{jj'}$ (i.e., $\mathbf{h} = \mathbf{h}^\dagger$ is Hermitean). Suppose that, at $t = t_0$, we diagonalize $\hat{H}(t_0)$ and find its eigenstates $u_{j\mu}$, which can be regarded as the columns of a unitary matrix $\mathbf{U}_0$, with increasing energy as the column index increases. The structure of the matrix $\mathbf{U}_0$ can be schematized as follows:

$$\mathbf{U}_0 = \left[\ \mathbf{F}_0 \ \middle|\ \mathbf{E}_0\ \right] , \tag{1.156}$$

where $\mathbf{F}_0$ is an $L \times N_p$ matrix, N_p being the number of particles, i.e., the number of *filled* eigenstates, while $\mathbf{E}_0$ is an $L \times (L - N_p)$ matrix containing the *empty* states. [24] The operator $\hat{a}^\dagger_\mu$ associated to the μ-th eigenstate is:

$$\hat{a}^\dagger_\mu = \sum_j u_{0j\mu}\hat{c}^\dagger_j = \sum_j \left[\mathbf{U}_0^T\right]_{\mu j}\hat{c}^\dagger_j \ .$$

In matrix form, this can be written as

$$\hat{\mathbf{a}}^\dagger = \mathbf{U}_0^T \cdot \hat{\mathbf{c}}^\dagger \qquad \Rightarrow \qquad \hat{\mathbf{c}} \ = \mathbf{U}_0 \cdot \hat{\mathbf{a}} \ . \tag{1.157}$$

To study the dynamical case, let us write the Heisenberg's equation of motion for the operator $\hat{c}_j$

$$i\hbar\frac{d}{dt}\hat{c}_{jH}(t) = \hat{U}^\dagger(t,t_0)\left[\hat{c}_j, \hat{H}(t)\right]\hat{U}(t,t_0) = \sum_{j'} h_{jj'}(t)\ \hat{c}_{j'H}(t) \ . \tag{1.158}$$

[23] Indeed, Thouless original derivation applies to Slater determinants, and not to general BCS-states.
[24] Although in principle $L = \infty$, in actual practice L is finite.

We search for a solution of the form:

$$\hat{\mathbf{c}}_H(t) = \mathbf{U}(t) \cdot \hat{\mathbf{a}} \ ,$$

where $\hat{\mathbf{a}}$ are the same operators diagonalizing $\hat{H}(t_0)$, and $\mathbf{U}(t)$ is a time-dependent unitary matrix satisfying the initial condition $\mathbf{U}(t_0) = \mathbf{U}_0$. It is straightforward to show that, in order to solve the Heisenberg equations for $\hat{\mathbf{c}}_H(t)$, the matrix $\mathbf{U}(t)$, which we again decompose as $\mathbf{U}(t) = \left[\ \mathbf{F}(t) \ \middle| \ \mathbf{E}(t) \ \right]$, has to satisfy:

$$i\hbar \frac{d}{dt}\mathbf{U}(t) = \mathbf{h}(t) \cdot \mathbf{U}(t) = \left[\ \mathbf{h}(t) \cdot \mathbf{F}(t) \ \middle| \ \mathbf{h}(t) \cdot \mathbf{E}(t) \ \right] . \tag{1.159}$$

Notice the similarity with the BdG equations, with an important difference (apart from an explicit factor 2 in the BdG equation which is missing here): $\mathbf{U}(t)$ is an $L \times L$ matrix, while $\mathbb{U}\ (t)$ was $2L \times 2L$, although in the end one can always study a $2L \times L$ BdG problem. Solving Eq. (1.159) with initial condition $\mathbf{U}(t_0) = \mathbf{U}_0$ is enough to calculate averages of operators. For instance, the Green's functions are given by:

$$\begin{aligned} G^h_{j'j}(t) &= \langle \psi(t_0) | \hat{c}^\dagger_{jH}(t) \hat{c}_{j'H}(t) | \psi(t_0) \rangle = \sum_{\mu=1}^{N_p} U^*_{j\mu}(t) U_{j'\mu}(t) = \Big[\mathbf{F}(t) \cdot \mathbf{F}^\dagger(t) \Big]_{j'j} \\ G^p_{j'j}(t) &= \langle \psi(t_0) | \hat{c}_{jH}(t) \hat{c}^\dagger_{j'H}(t) | \psi(t_0) \rangle = \sum_{\mu>N_p} U_{j\mu}(t) U^*_{j'\mu}(t) = \Big[\mathbf{E}^*(t) \cdot \mathbf{E}^T(t) \Big]_{j'j} \end{aligned} \tag{1.160}$$

where the superscript h/p in $G_{j'j}$ refer to the hole/particle case. A further reduction of computation cost occurs if one is interested only in quantities that depend on the occupied orbitals only, i.e., on $\mathbf{F}(t)$. The equation for $\mathbf{F}(t)$ is indeed an $L \times N_p$ system:

$$i\hbar \frac{d}{dt}\mathbf{F}(t) = \mathbf{h}(t) \cdot \mathbf{F}(t) \ , \tag{1.161}$$

with initial condition $\mathbf{F}(t_0) = \mathbf{F}_0$.

The final point of our discussion is how the Slater determinant $|\psi(t)\rangle$ at time t is related to the initial Slater determinant $|\psi(t_0)\rangle$, i.e., the Thouless formula. Going back to the Scrödinger picture, we have:

$$\hat{\mathbf{a}} \ = \mathbf{U}^\dagger(t) \cdot \hat{\mathbf{c}}_H(t) \qquad \Rightarrow \qquad \hat{\mathbf{a}}(t) = \mathbf{U}^\dagger(t) \cdot \hat{\mathbf{c}} \ ,$$

or, with explicit indices:

$$\hat{a}^\dagger_\mu(t) = \sum_j U_{j\mu}(t) \ \hat{c}^\dagger_j \ . \tag{1.162}$$

The operators $\hat{a}_\mu(t)$ are such that, by construction, they annihilate $|\psi(t)\rangle$ for $\mu = 1 \cdots N_p$, at any time t, i.e.:

$$|\psi(t_0)\rangle = \prod_{\mu=1}^{N_p} \hat{a}^\dagger_\mu |0\rangle \quad \text{and} \quad |\psi(t)\rangle = \prod_{\mu=1}^{N_p} \hat{a}^\dagger_\mu(t) |0\rangle \ . \tag{1.163}$$

Substituting Eq. (1.162) one can write, at any time t:

$$|\psi(t)\rangle = \sum_{j_1<j_2<\cdots<j_{N_p}} \det[\mathbf{F}(t)]_{j_1 \cdots j_{N_p}} \ \hat{c}^\dagger_{j_1} \cdots \hat{c}^\dagger_{j_{N_p}} |0\rangle \ , \tag{1.164}$$

where $\det[\mathbf{F}(t)]_{j_1\cdots j_{N_p}}$ is the $N_p \times N_p$-minor of $\mathbf{F}(t)$ extracted taking the rows $j_1 \cdots j_{N_p}$. The latter expression tells us the Slater determinant $|\psi(t)\rangle$ in terms of the vacuum $|0\rangle$, and is not the Thouless formula we are looking for, expressing $|\psi(t)\rangle$ in terms of $|\psi(t_0)\rangle$.

The Thouless formula derives from appreciating that there is a direct unitary transformation between $\hat{\mathbf{a}}(t)$ and $\hat{\mathbf{a}}$ which reads:

$$\hat{\mathbf{a}}(t) = \mathbf{U}^\dagger(t)\cdot\hat{\mathbf{c}} = \underbrace{\mathbf{U}^\dagger(t)\cdot\mathbf{U}_0}_{\stackrel{def}{=}\mathbf{U}_t^\dagger}\cdot\hat{\mathbf{a}} \quad \Rightarrow \quad \hat{\mathbf{a}}^\dagger(t) = \mathbf{U}_t^T\cdot\hat{\mathbf{a}}^\dagger \,. \tag{1.165}$$

Written explicitly, the unitary transformation $\mathbf{U}_t$ is given by:

$$\mathbf{U}_t = \mathbf{U}_0^\dagger\cdot\mathbf{U}(t) = \left[\begin{array}{c|c} \mathbf{F}_0^\dagger\cdot\mathbf{F}(t) & \mathbf{F}_0^\dagger\cdot\mathbf{E}(t) \\ \hline \mathbf{E}_0^\dagger\cdot\mathbf{F}(t) & \mathbf{E}_0^\dagger\cdot\mathbf{E}(t) \end{array}\right] \quad \Rightarrow \quad \mathbf{U}_t^T = \left[\begin{array}{c|c} \mathbf{F}^T(t)\cdot\mathbf{F}_0^* & \mathbf{F}^T(t)\cdot\mathbf{E}_0^* \\ \hline \mathbf{E}^T(t)\cdot\mathbf{F}_0^* & \mathbf{E}^T(t)\cdot\mathbf{E}_0^* \end{array}\right] . \tag{1.166}$$

We now observe that the $N_p \times N_p$ matrix $\mathbf{Q}(t) = \mathbf{F}^T(t)\cdot\mathbf{F}_0^*$ is invertible [25] and therefore we can define new operators

$$\hat{\mathbf{b}}^\dagger(t) = \left[\begin{array}{c|c} \mathbf{Q}^{-1}(t) & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{1} \end{array}\right]\cdot\hat{\mathbf{a}}^\dagger(t) = \left[\begin{array}{c|c} \mathbf{1} & \mathbf{Z}(t) \\ \hline \mathbf{E}^T(t)\cdot\mathbf{F}_0^* & \mathbf{E}^T(t)\cdot\mathbf{E}_0^* \end{array}\right]\cdot\hat{\mathbf{a}}^\dagger \,, \tag{1.167}$$

where $\mathbf{Z}(t) = \mathbf{Q}^{-1}(t)\cdot\mathbf{F}^T(t)\cdot\mathbf{E}_0^*$. [26] Using these new operators, one can write an explicit expression for the occupied orbital indices $\mu = 1\cdots N_p$ in the form:

$$\hat{b}^\dagger_{\mu<N_p}(t) = \hat{a}^\dagger_{\mu<N_p} + \sum_{\mu'>N_p}[\mathbf{Z}(t)]_{\mu\mu'}\hat{a}^\dagger_{\mu'} \,. \tag{1.168}$$

And now comes the final crucial observation that, since the occupied $\hat{b}^\dagger_\mu(t)$ are simply a mixture of the occupied $\hat{a}^\dagger_\mu(t)$, we can equivalently express the Slater determinant as:

$$\begin{aligned} |\psi(t)\rangle &= \prod_{\mu=1}^{N_p}\hat{b}^\dagger_\mu(t)\,|0\rangle \\ &= \prod_{\mu=1}^{N_p}\Big[\hat{a}^\dagger_\mu + \sum_{\mu'>N_p}[\mathbf{Z}(t)]_{\mu\mu'}\hat{a}^\dagger_{\mu'}\hat{a}_\mu\hat{a}^\dagger_\mu\Big]|0\rangle = \prod_{\mu=1}^{N_p}\Big[\Big(1+\sum_{\mu'>N_p}[\mathbf{Z}(t)]_{\mu\mu'}\hat{a}^\dagger_{\mu'}\hat{a}_\mu\Big)\hat{a}^\dagger_\mu\Big]|0\rangle \\ &= \exp\Big(\sum_{\mu=1}^{N_p}\sum_{\mu'>N_p}[\mathbf{Z}(t)]_{\mu\mu'}\hat{a}^\dagger_{\mu'}\hat{a}_\mu\Big)\prod_{\mu=1}^{N_p}\hat{a}^\dagger_\mu\,|0\rangle \\ &= \exp\Big(\sum_{\mu=1}^{N_p}\sum_{\mu'>N_p}[\mathbf{Z}(t)]_{\mu\mu'}\hat{a}^\dagger_{\mu'}\hat{a}_\mu\Big)\,|\psi(t_0)\rangle \,, \end{aligned} \tag{1.169}$$

which is the desired Thouless formula.

[25] Explain why.

[26] One would be tempted to write an explicit expression for $\mathbf{Q}^{-1}$ in the form $[\mathbf{F}_0^*]^{-1}\cdot[\mathbf{F}^T(t)]^{-1}$, which would then lead to $\mathbf{Z}(t) = [\mathbf{F}_0^*]^{-1}\cdot\mathbf{E}_0^*$, independent of t. This is, however, wrong, because the matrix $\mathbf{F}$ is not a square matrix, and cannot be inverted. What is easy to prove is that, at time $t = t_0$, we have $\mathbf{Q}(t_0) = \mathbf{1}$, hence $\mathbf{Z}(t_0) = \mathbf{F}_0^T\cdot\mathbf{E}_0^* = \mathbf{0}$, because of the orthogonality of empty and occupied states.

Part II.

Floquet systems

2. Floquet and tight-binding systems

The plan/summary of this Chapter is the following. We start by reviewing the Floquet theorem for time-periodic Hamiltonians $\hat{H}(t) = \hat{H}(t+\tau)$. This theorem generalizes a well-know fact of quantum mechanics: if $\hat{H}$ does not depend on t, then you can find its eigenstates $|\phi_\alpha\rangle$ and the associated energies E_α and, in terms of them, express the evolution operator as:

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar} = \sum_\alpha e^{-iE_\alpha t/\hbar} |\phi_\alpha\rangle\langle\phi_\alpha| \, .$$

Floquet theorem guarantees that, if $\hat{H}(t+\tau) = \hat{H}(t)$ with some period τ then:

$$\hat{U}(t,0) = \sum_\alpha e^{-i\mu_\alpha t/\hbar} |\phi_\alpha(t)\rangle\langle\phi_\alpha(0)| \, ,$$

where the states $|\phi_\alpha(t)\rangle$ are *periodic*, and form a complete set. Moreover, one establishes also that $\hat{U}(t+n\tau,0) = \hat{U}(t,0)\hat{U}^n(\tau,0)$. Next I derive and discuss the Standard Map for a periodically kicked pendulum, one of the easiest examples of classical chaos in one-dimensional driven systems, showing that the probability distribution of momentum, in the chaotic regime, is a Gaussian which broadens in the way which is characteristic of Brownian motion and classical diffusion. Finally, we apply the Floquet machinery to discuss the quantum version of the same Hamiltonian, discussing the mechanism behind a suppression of diffusion due to quantum interference that goes under the name of *dynamical localization*.

2.1. Time-periodic Hamiltonians: The Floquet theorem

There are many proofs of Floquet theorem: the one I reproduce here mimicks, I believe, the original Floquet-Lyapunov analysis of the stability of the linearized motion around a periodic orbit solution (see for instance the book by Gantmakher, *Theory of Matrices*). We take here, for convenience, $\hbar = 1$ and abandon, for a while, the ket notation for quantum states, in favor of a vector notation, for which we will make a **bold** use of boldface types. The Schrödinger equation (SE) reads:

$$i\dot{\boldsymbol{\psi}}(t) = \mathbf{H}(t) \cdot \boldsymbol{\psi}(t) \, , \tag{2.1}$$

with a given initial condition at time $t = 0$: $\boldsymbol{\psi}(0) = \boldsymbol{\psi}_0$. As well known from Quantum Mechanics, one can formally solve the dynamics by introducting a propagator $\mathbf{U}(t,0)$ such that $\boldsymbol{\psi}(t) = \mathbf{U}(t,0)\cdot\boldsymbol{\psi}_0$ (this is a consequence of the linearity of the problem), where $\mathbf{U}(0,0) = \mathbb{1}$ to account for the initial value condition. [1] Take now, as initial value states, a complete

[1] The basic properties of $\mathbf{U}$ are that $\mathbf{U}$ is unitary (because $\mathbf{H}$ is Hermitean) and that $\mathbf{U}(t'',t')\cdot\mathbf{U}(t',t) = \mathbf{U}(t'',t)$. Both properties are true quite generally even for time-dependent Hamiltonians.

basis set of orthonormal states of the Hilbert state, and collect all such $\boldsymbol{\psi}_0$ as column vectors of a "matrix" $\boldsymbol{\Psi}_0$ (in general this is an ∞-dimensional matrix) which is unitary since its columns are *orthonormal* vectors. In the same spirit, collect all solutions of the SE Eq. (2.1) starting from such a basis of initial values into a "matrix" $\boldsymbol{\Psi}(t)$ which will obviously satisfy:

$$i\dot{\boldsymbol{\Psi}}(t) = \mathbf{H}(t) \cdot \boldsymbol{\Psi}(t) \ , \tag{2.2}$$

with initial condition $\boldsymbol{\Psi}(0) = \boldsymbol{\Psi}_0$. [2] The reason why one does that will be more clear in a second. Since the propagator is unitary, it conserves scalar products between states, which immediately implies that $\boldsymbol{\Psi}(t)$ is also unitary (its colums are orthonormal vectors at any time t). In terms of the propagator we therefore have:

$$\boldsymbol{\Psi}(t) = \mathbf{U}(t,0) \cdot \boldsymbol{\Psi}_0 \ , \tag{2.3}$$

where all the objects appearing are unitary. Until now we have not assumed periodicity of the Hamiltonian. Assume now that $\mathbf{H}(t+\tau) = \mathbf{H}(t)$ with some period τ, and consider the states $\boldsymbol{\Phi}(t) = \boldsymbol{\Psi}(t+\tau)$. It is a simple matter to prove that $\boldsymbol{\Phi}(t)$ obeys exactly the same SE in Eq. (2.2):

$$i\dot{\boldsymbol{\Phi}}(t) = i\dot{\boldsymbol{\Psi}}(t+\tau) = \mathbf{H}(t+\tau) \cdot \boldsymbol{\Psi}(t+\tau) = \mathbf{H}(t) \cdot \boldsymbol{\Psi}(t+\tau) = \mathbf{H}(t) \cdot \boldsymbol{\Phi}(t) \ .$$

And here comes the usefulness of having worked with matrices that embody *all possible linearly independent* solutions of the SE, and not just a single one. Indeed, if $\boldsymbol{\Phi}(t)$ obeys the same equation as $\boldsymbol{\Psi}(t)$, then there must exsist some other initial value $\boldsymbol{\Psi}'_0$ such that $\boldsymbol{\Phi}(t) = \mathbf{U}(t,0) \cdot \boldsymbol{\Psi}'_0$. This is so because *all* solutions of the SE in matrix form should necessarily be of that form. Indeed, putting $t = 0$ and recalling that $\boldsymbol{\Phi}(0) = \boldsymbol{\Psi}(\tau)$ and that $\mathbf{U}(0,0) = \mathbb{1}$ we immediately deduce that $\boldsymbol{\Psi}'_0 = \boldsymbol{\Psi}(\tau)$. Therefore, we have just deduced that: $\boldsymbol{\Psi}(t+\tau) = \mathbf{U}(t,0) \cdot \boldsymbol{\Psi}(\tau) = \mathbf{U}(t,0) \cdot \mathbf{U}(\tau,0) \cdot \boldsymbol{\Psi}_0$, which, together with the always valid relationship $\boldsymbol{\Psi}(t+\tau) = \mathbf{U}(t+\tau,0) \cdot \boldsymbol{\Psi}_0$, implies the following identity:

$$\mathbf{U}(t+\tau,0) = \mathbf{U}(t,0) \cdot \mathbf{U}(\tau,0) \ . \tag{2.4}$$

Notice that, on general grounds, you would have split the propagation from 0 to $t+\tau$ as

$$\mathbf{U}(t+\tau,0) = \mathbf{U}(t+\tau,\tau) \cdot \mathbf{U}(\tau,0) \ .$$

Therefore, what we have just proved can be rephrased by saying that $\mathbf{U}(t+\tau,\tau) = \mathbf{U}(t,0)$: in words, the propagation by t starting from time τ coincides with the same propagation starting from time 0. [3] The proof now goes on along lines which you can easily anticipate. Consider $\boldsymbol{\Phi}(t) = \boldsymbol{\Psi}(t+n\tau)$ and again prove that is satisfies the same SE as $\boldsymbol{\Psi}(t)$, which almost immediately leads you to write that $\mathbf{U}(t+n\tau,0) = \mathbf{U}(t,0) \cdot \mathbf{U}(n\tau,0)$. An easily constructed induction-proof leads, finally, to the following important relationship:

$$\mathbf{U}(t+n\tau,0) = \mathbf{U}(t,0) \cdot [\mathbf{U}(\tau,0)]^n \ . \tag{2.5}$$

It is obvious that, although the previous equation is true for any value of t, you can restrict t to $t \in [0,\tau]$: $n\tau$ is the multiple of the period which is closest to the final propagation time,

[2] In the classical Floquet-Lyapunov theory of first-order linear time-periodic systems, $\boldsymbol{\Psi}(t)$ is usually called a *matrix integral*.

[3] This should not induce you to believe that $\mathbf{U}(t',t)$ depends on $t'-t$: it doesn't. Neither you should believe that, for instance, $\mathbf{U}(t+\tau,t) = \mathbf{U}(\tau,0)$, which is *wrong*.

and t is the residual time within the $(n+1)$-th period. The practical value of Eq. (2.5) is immense: you can propagate a state up to an arbitrary large time $t + n\tau$ by just knowing $\mathbf{U}(\tau, 0)$ (which is applied n times) and $\mathbf{U}(t, 0)$ with $t < \tau$. [4]

This ends the first part of the story on the Floquet theorem. Now comes an equally useful and important second part. First of all, the important actor in the game is evidently $\mathbf{U}(\tau, 0)$, the propagator over one period, sometimes called the *Floquet* operator. [5] If you know how to integrate, for instance numerically, your SE for a time τ you can obtain $\mathbf{U}(\tau, 0)$ as the time-evolved state matrix $\mathbf{\Psi}(\tau)$ with initial condition $\mathbf{\Psi}(0) = \mathbb{1}$. Indeed: $\mathbf{\Psi}(\tau) = \mathbf{U}(\tau, 0) \cdot \mathbf{\Psi}(0) = \mathbf{U}(\tau, 0)$. Now, every unitary operator can be diagonalized by a unitary matrix. [6] Therefore, there must exist a complete set of states $\boldsymbol{\phi}_\alpha$ such that

$$\mathbf{U}(\tau, 0) \cdot \boldsymbol{\phi}_\alpha = \lambda_\alpha \boldsymbol{\phi}_\alpha = e^{-i\mu_\alpha \tau} \boldsymbol{\phi}_\alpha \,, \tag{2.6}$$

where we have used the fact that the complex eigenvalues λ_α lie on the unit circle in the complex plane, $|\lambda_\alpha| = 1$, and we have introduced the phases μ_α by extracting (for later convenience) a τ. Collecting all the μ_i in a diagonal matrix $\boldsymbol{\mu}$, and all the eigenvectors $\boldsymbol{\phi}_\alpha$ as column vectors of a (unitary) matrix $\mathbf{\Phi}$ we can rewrite the eigenvalue problem as:

$$\mathbf{U}(\tau, 0) \cdot \mathbf{\Phi} = \mathbf{\Phi} \cdot e^{-i\boldsymbol{\mu}\tau} \qquad \Longrightarrow \qquad \mathbf{U}(\tau, 0) = \mathbf{\Phi} \cdot e^{-i\boldsymbol{\mu}\tau} \cdot \mathbf{\Phi}^\dagger \,. \tag{2.7}$$

Notice that the matrix multiplication rules force you to write the diagonal term $e^{-i\boldsymbol{\mu}\tau}$, in the first expression, to the *right* of the eigenvector matrix $\mathbf{\Phi}$: if you put it to the left, it does not work! The $\mathbf{\Phi}$ and the $\boldsymbol{\mu}$ just introduced, eigenvectors and phases of the unitary operator $\mathbf{U}(\tau, 0)$, are very important: they are called *Floquet modes* (the $\mathbf{\Phi}$) and *Floquet quasi-energies* (the $\boldsymbol{\mu}$). And now comes the final piece of the story. Look again at the eigenvalue problem defining $\mathbf{\Phi}$, $\mathbf{U}(\tau, 0) \cdot \mathbf{\Phi} = \mathbf{\Phi} \cdot e^{-i\boldsymbol{\mu}\tau}$: it tells us that, by evolving over a full period τ, the states $\mathbf{\Phi}$ get multiplied by a phase factor $e^{-i\boldsymbol{\mu}\tau}$. Consider now $\mathbf{U}(t, 0) \cdot \mathbf{\Phi}$ for $t \leq \tau$. By a seemingly trivial manipulation, write it as:

$$\mathbf{U}(t, 0) \cdot \mathbf{\Phi} = \underbrace{\mathbf{U}(t, 0) \cdot \mathbf{\Phi} \cdot e^{+i\boldsymbol{\mu}t}}_{\mathbf{\Phi}(t)} \cdot e^{-i\boldsymbol{\mu}t} = \mathbf{\Phi}(t) \cdot e^{-i\boldsymbol{\mu}t} \,, \tag{2.8}$$

where the newly defined quantity

$$\mathbf{\Phi}(t) \stackrel{def}{=} \mathbf{U}(t, 0) \cdot \mathbf{\Phi} \cdot e^{+i\boldsymbol{\mu}t} \,, \tag{2.9}$$

is time-periodic because $\mathbf{\Phi}(\tau) = \mathbf{\Phi}(0) = \mathbf{\Phi}$. Eq. (2.8) is the promised result: we have found a complete set of states $\mathbf{\Phi}$, the Floquet modes, which evolve with a time-periodic part $\mathbf{\Phi}(t)$ times a phase factor $e^{-i\boldsymbol{\mu}t}$. Equivalently, we can rewrite Eq. (2.9) in the form:

$$\mathbf{U}(t, 0) = \mathbf{\Phi}(t) \cdot e^{-i\boldsymbol{\mu}t} \cdot \mathbf{\Phi}^\dagger(0) \,, \tag{2.10}$$

[4] Notice, once again, that the order is important. It would be *wrong* to write something like $\mathbf{U}(t + n\tau, 0) = [\mathbf{U}(\tau, 0)]^n \cdot \mathbf{U}(t, 0)$.

[5] In the derivation of Stöckmann, $\mathbf{U}(\tau, 0)$ is just the unitary operator T_τ that performs a time-translation by one period, and which can be diagonalized by the Floquet modes while still solving the Schrödinger equation, see explicit proof below.

[6] Indeed, any *normal* operator, i.e., such that $A^\dagger A = A A^\dagger$ can be diagonalized by a unitary operator V, writing $A = V Diag[\lambda_\alpha] V^\dagger$. In particular, this implies that unitary operators and Hermitean operators can be both be diagonalized by a unitary operator.

which holds true for any t, and even adventure in proving (easy) that:

$$\mathbf{U}(t,t') = \mathbf{\Phi}(t) \cdot e^{-i\boldsymbol{\mu}(t-t')} \cdot \mathbf{\Phi}^\dagger(t') \; . \tag{2.11}$$

Summarizing: 1) if we are able to construct $\mathbf{U}(t,0)$ for all $t \in [0,\tau]$, then we have all the information we need to carry out an arbitrary long time-propagation; 2) the eigenstates $\mathbf{\Phi}$ of $\mathbf{U}(\tau,0)$, and the corresponding eigenvalues phases $\boldsymbol{\mu}$, give us states which propagate as a periodic part $\mathbf{\Phi}(t)$ times a phase factor $e^{-i\boldsymbol{\mu}t}$. [7]

2.2. Dynamical localization

2.2.1. The kicked pendulum

The solutions of the periodically driven pendulum outside the region of stability of the linear Mathieu problem are evidently solutions that starts growing and likely display chaotic behaviour, except that they loose any meaning as soon as θ starts growing: in reality, the non-linearity of the $\sin\theta$ term is crucial to describe such chaotic behaviour. If we want to keep the non-linear term we have to pay some price and simplify the equation. To that purpose, consider a rather peculiar driven pendulum in which $g(t)$ is mostly 0 except at periodic intervals of time, in which it is a δ-function:

$$g(t) = g\, \delta_P(t/\tau) \stackrel{def}{=} g \sum_n \delta(t/\tau - n) = g\tau \sum_n \delta(t - n\tau) \; , \tag{2.13}$$

where the second expression comes from recalling that $\delta(t/\tau - n) = \tau\delta(t - n\tau)$. This equation defines the periodic delta-function $\delta_P(t/\tau)$. Notice that here τ is the period between the kicks but also serves as a coupling strength for the kicks. You might be worried by such a singular shape, but you should be amply accustomed to such extreme (impulsive) forces since the early days of your study of mechanics: a collision of a particle on a wall is usually thought to have a neagligeably small duration Δt, during which the (impulsive) force $F(t)$ due to the wall becomes very large in such a way that the integral $\int_{t_0}^{t_0+\Delta t} dt F(t) = I$ remains finite: by assuming $\Delta t \to 0$ we are in practice assuming that the $F(t)$ has a singular delta-function nature $F(t) = I\delta(t - t_0)$. Nothing really upsets us so much: the important thing is that we can meaningfully calculate, from $\dot{p} = F(t)$, the finite change in momentum $\Delta p = p(t_0+\epsilon) - p(t_0) = I$. Here, as well, you can think of the $g(t)$ giving sharp, large but finite kicks in a small time-interval Δt, with time-integral $g\tau$, and then take $\Delta t \to 0$ keeping τ finite. Having understood that, let us write the Hamiltonian of the kicked pendulum as:

$$H_{\rm kp}(\theta, p_\theta, t) = \frac{p_\theta^2}{2ml^2} - mlg\, \delta_P(t/\tau) \cos\theta \; . \tag{2.14}$$

from which the following Hamilton's equations follow immediately:

$$\begin{aligned} \dot{\theta} &= \frac{p_\theta}{ml^2} \\ \dot{p}_\theta &= -mlg\, \delta_P(t/\tau) \sin\theta \; . \end{aligned} \tag{2.15}$$

[7] For those of you who cannot renounce to the Dirac notation, here is how Eq. (2.10) looks like with bras and kets:

$$\mathbf{U}(t,0) = \sum_\alpha e^{-i\mu_\alpha t} |\boldsymbol{\phi}_\alpha(t)\rangle\langle\boldsymbol{\phi}_\alpha(0)| \; . \tag{2.12}$$

So, $p_\theta(t)$ is piece-wise constant in time, with jumps at time $t = n\tau$ from some value $p(n\tau-\epsilon) = p_n^-$ to a new value $p(n\tau+\epsilon) = p_n^+$. $\theta(t)$ is piece-wise linear and continuous, with discontinuities only in the slope. Defining $\theta_n = \theta(n\tau)$ and integrating the equations from $t = n\tau - \epsilon$ to $t = (n+1)\tau - \epsilon$ we get:

$$\begin{aligned} \theta_{n+1} - \theta_n &= \frac{p_n^+}{ml^2}\tau \\ p_n^+ - p_n^- &= -mlg\tau \sin\theta_n \ . \end{aligned} \tag{2.16}$$

Now define a dimensionless (angular) momentum as $L_n = \tau p_n^-/(ml^2) = \tau p_\theta(n\tau - \epsilon)/(ml^2)$ and observe that L_{n+1} is also related to the value of p_n^+, which is conserved in the interval $[n\tau + \epsilon, (n+1)\tau - \epsilon]$. Therefore, we can write the equations as: Standard map

$$\begin{aligned} \theta_{n+1} &= \theta_n + L_{n+1} \\ L_{n+1} &= L_n - K\sin\theta_n \ , \end{aligned} \tag{2.17}$$

where we have defined the dimensionless kick-strength $K = g\tau^2/l = \omega_0^2\tau^2$. Notice also that time is now measured in units of the period τ. Eq. (2.17) defines a *discrete map* in phase space (θ, p_θ), known as *standard map*, or Chirikov map. Formally, we have:

$$(\theta_{n+1}, L_{n+1}) = Z_K(\theta_n, L_n) \ . \tag{2.18}$$

Obviously, a similar equation might have been written for the periodically driven pendulum, because the values of θ and p_θ at time $t = n\tau$ *univocally determine* their values at time $t = (n+1)\tau$: the difficulty with a general periodically driven pendulum is that the map itself has to be constructed numerically, in general, which makes the analysis of the chaotic behaviour much more cumbersome. On the contrary, by trading the regular periodic driving with a singular kicked driving we have been able to construct the discrete map Z_K analytically, with very little effort. Similar maps, generally known as Poincaré maps, are often constructed to analyse continuous-time dynamical systems in a simplified way. [8] A few comments about the relevant region in phase space are essential. First, notice that you can always restrict θ in a 2π interval, for instance $\theta \in [-\pi, \pi)$, and write the first equation as $\theta_{n+1} = (\theta_n + L_{n+1}) \mod(2\pi)$. L in principle can assume any value, and increase without bounds. However, because of the $\mod(2\pi)$ restriction in the equation for θ, we can always fold back whatever value we have of L_{n+1} into a $[-\pi, \pi)$ region as well. Therefore, we can safely plot the map in the finite region $[-\pi, \pi) \times [-\pi, \pi)$, although the actual dynamics of L_n has to be kept track of in analysing, for instance, the evolution of the total kinetic energy L_n^2 at time $n\tau$. We will discuss this point later on, showing a crucial difference between classical and quantum dynamics in that respect: quantum dynamics shows a phenomenon called *dynamical localization*, which is absent in classical physics. Returning to the standard map, we plot iterations of the map for different values of K in Fig. 2.1. To fix the ideas, suppose you have the non-interacting map with $K = 0$ (no kicks): Z_0. This simply gives:

$$\begin{aligned} \theta_{n+1} &= \theta_n + L_{n+1} \\ L_{n+1} &= L_n \ , \end{aligned} \tag{2.19}$$

[8] Often the Poincaré map is constructed not by a stroboscopic observation of the system at discrete times $n\tau$, but rather by observing the points reached by the evolution on a certain 2-dimensional manifold in phase space, known as Poincaré section.

i.e., L is conserved by the map (in Hamiltonian mechanics of integrable systems you would call it the *action variable*), while θ_n increases in a simple way: if L denotes the conserved value of the momentum, then $\theta_n = \theta_0 + nL$. So the θ (called the *angle variable*) increases linearly with time at a rate controlled by L. Now you appreciate easily that if L is a *rational* multiple of 2π, i.e., $L = 2\pi n/k$ with n and k integers, then $\theta_k = \theta_0 + k(2\pi n/k) = \theta_0 + 2\pi n = \theta_0$, i.e., the map periodically repeates itself after k steps, k being the denominator in the rational $L/(2\pi)$: by iterating the map from an initial point θ_0 you will get only a finite numeber, k, of points. On the contrary, if $L/(2\pi)$ is irrational, then the θ_n fill uniformly the region $[-\pi, \pi]$ without ever returning to the same point: by iterating the map you will get a straight segment densily filled with points: these are the irrational *invariant Tori*. Now, a theorem due to Poincaré and Birkhoff shows that the rational values of L are very fragile to perturbations, and adding even a small K breaks them into an alternation of hyperbolic and elliptic points (see José&Saletan, for instance). On the contrary, the famous KAM theorem guarantees that the most irrational Tori survive perturbation, until, when the last of them gives up upon increasing K beyond some critical value K_c, full chaos develops. Without pretending having explained KAM theorem, let us give a look at the results of iterating the Standard Map, shown in Fig. 2.1 (in class I showed animations, due to Simone Ziraldo, which illustrate the dynamics in a more clear way). In each plot, the initial values of L_0 are 62 equispaced points in the iterval $[-\pi, \pi]$ (so, very rational multiples of 2π), while the corresponding initial values of θ_0, for each L_0, are 62 randomly chosen points: then the map is let evolve for $n = 1000$ iterations, and all points obtained are drawn in the diagram (shifting, whenever necessary, L_n by the appropriate multiple of 2π so that L_n is visualized in $[-\pi, \pi]$) Notice first, for $K = 0$, the trajectories consisting of a finite number k of points, the k of the denominator of $L = 2\pi n/k$. Next, Notice that for low values of K the "trajectories" followed by the map are essentially gently curved almost horizontal lines (invariant Tori of the map), with a few regions associated to closed orbits around some points (elliptic points) and saddle orbits around other (hyperbolic points), which originate from breaking of the invariant Tori for most rational values of L. A full discussion of this is given, for instance, in the book by José and Saletan. It suffices here to say that for values of $K < K_c \approx 0.9716$ surviving Tori exist (look at the $K = 0.75$ plot) which run horizontally although in a gently curved way: due to a uniqueness-theorem for the map iteration, no trajectory can ever cross those "highways", which behave as impenetrable fences for the "sheeps" inside: therefore, the values of L cannot go wildly large. For $K > K_c$ the last surviving Torus has given up and L can increase without bounds, in a kind of Brownian way (see below), leading to an increase in kinetic energy roughly linear in n: the fences are gone and the "sheeps" diffuse away all around.

Let us give here an argument showing that, for $K \gg K_c$ one expects $\langle L^2 \rangle_n \sim Dn$ with a diffusion constant $D = K^2/2$. Suppose you iterate the Standard Map by starting from $L_0 = 0$ but in the deeply chaotic regime $K \gg K_c$. Given some initial θ_0 you will get:

$$\begin{aligned} L_1 &= -K \sin\theta_0 && \longrightarrow \theta_1 = \theta_0 + L_1 \\ L_2 &= -K \sin\theta_0 - K \sin\theta_1 && \longrightarrow \theta_2 = \theta_1 + L_2 \\ &\cdots \\ L_n &= -K \textstyle\sum_{j=0}^{n-1} \sin\theta_i \end{aligned} \tag{2.20}$$

Due to the large value of the kick parameter K, one can easily appreciate that the various θ_j

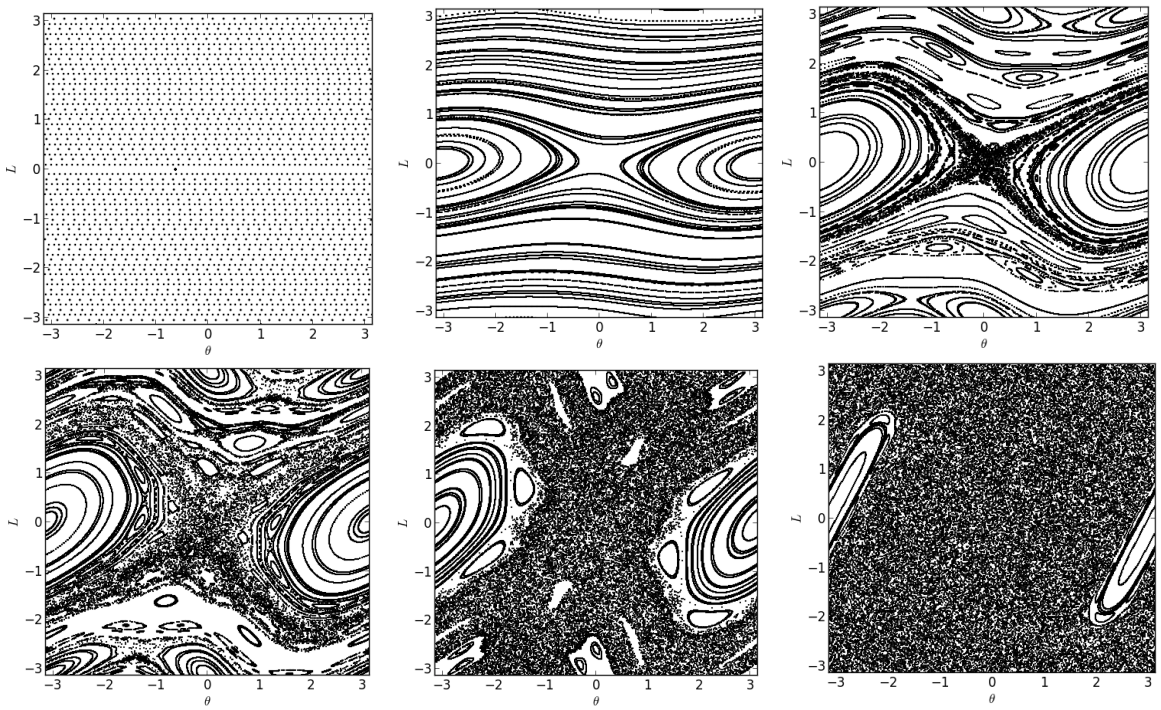

Figure 2.1.: Standard map iterations for increasing values of k (from top left to bottom right): $K = 0, 0.25, 0.75, 1, 1.5, 4$. For each K, the initial values of L_0 where 62 equispaced points in $[-\pi, \pi)$, while the corresponding initial values of θ_0 where selected randomly in $[\pi, \pi)$. The map has been iterated for $n = 1000$ steps for each of the 62 initial values of (θ_0, L_0).

are largely uncorrelated one from the other! Therefore, if I evaluate the average L_n^2 I get:

$$\langle L_n^2 \rangle = \langle K^2 \sum_{j=0}^{n-1} \sum_{j'=0}^{n-1} \sin\theta_j \sin\theta_{j'} \rangle \approx K^2 \sum_{j=0}^{n-1} \langle \sin^2\theta_j \rangle \approx \frac{K^2}{2} n = Dn \ , \tag{2.21}$$

where we have disregarded correlations $\langle \sin\theta_j \sin\theta_{j'\neq j} \rangle \approx 0$, and assumed that all θ_j eventually cover uniformly the interval $[-\pi, \pi]$, i.e., $\langle \sin^2\theta_j \rangle = 1/2$. You should recognize here the *law of large numbers*, leading, via the *central limit theorem*, to the expectation that the distribution function of L at time n, $f_n(L)$, will be, for large n, a Gaussian with a second moment increasing as Dn. Indeed, with the same assumptions used above, we can calculate the distribution of angular momenta when one starts from $L_0 = 0$:

$$\begin{aligned} f_n(L) &= \langle \delta(L - L_n) \rangle = \langle \int_{-\infty}^{+\infty} \frac{dt}{2\pi} \, e^{it(L-L_n)} \rangle = \langle \int_{-\infty}^{+\infty} \frac{dt}{2\pi} \, e^{itL} \prod_{j=0}^{n-1} e^{iKt\sin\theta_j} \rangle \\ &\approx \int_{-\infty}^{+\infty} \frac{dt}{2\pi} \, e^{itL} \prod_{j=0}^{n-1} \langle e^{iKt\sin\theta_j} \rangle \approx \int_{-\infty}^{+\infty} \frac{dt}{2\pi} \, e^{itL} \prod_{j=0}^{n-1} [J_0(Kt)]^n \\ &\approx \int_{-\infty}^{+\infty} \frac{dt}{2\pi} \, e^{itL} e^{-nK^2t^2/4} = \frac{1}{\sqrt{\pi K^2 n}} e^{-L^2/(K^2 n)} \ . \end{aligned} \tag{2.22}$$

In the derivation we have used that:

$$\langle e^{iKt\sin\theta_j} \rangle \approx \int_0^{2\pi} \frac{d\theta}{2\pi} e^{iKt\sin\theta} = J_0(Kt) \ ,$$

and also that $[J_0(Kt)]^n$ is dominated, for large n, from the region of small Kt where it is legitimate to expand $J_0(Kt) = 1 - K^2t^2/t$. Writing $[J_0(Kt)]^n \approx e^{n\log(1-K^2t^2/4)}$ and expanding the log leads you to the goal.

2.2.2. The quantum kicked pendulum

Consider now the quantum version of the periodically kicked pendulum. Its Hamiltonian reads:

$$\hat{H}_{\rm kp}(t) = \frac{\hat{p}_\theta^2}{2ml^2} - mlg \ \delta_P(t/\tau)\cos\theta \ , \tag{2.23}$$

but now

$$\hat{p}_\theta = -i\hbar \frac{\partial}{\partial\theta} = \hbar \hat{L} \ ,$$

is an operator, which we have rewritten in terms of the dimensioness angular momentum. This Hamiltonian is an example of a class of periodically-kicked problems that you might write as:

$$\hat{H}_{\rm p-kick}(t) = \hat{T} + \delta_P(t/\tau) \ \hat{V} \ , \tag{2.24}$$

where $\hat{T}$ is the kinetic energy, and $\hat{V}$ the potential energy. To define the evolution operator over one period $\mathbf{U}(\tau, 0)$ it is convenient to regularize the δ-function by taking $\delta_P(t/\tau)$ to be 0 in the interval $[0, \tau - \Delta t]$ and $\tau/(\Delta t)$ in the interval $[\tau - \Delta t, \tau]$: the limit $\Delta t \to 0$ taken at the end. With this regularization the propagation is exactly expressed in terms of time-independent evolution operators as follows:

$$\mathbf{U}(\tau, 0) = \lim_{\Delta t \to 0} e^{-\frac{i}{\hbar}(\hat{T} + \frac{\tau}{\Delta t}\hat{V})\Delta t} e^{-\frac{i}{\hbar}\hat{T}(\tau - \Delta t)} = e^{-\frac{i}{\hbar}\hat{V}\tau} e^{-\frac{i}{\hbar}\hat{T}\tau} \ . \tag{2.25}$$

This holds quite generally for any $\hat{T}$ and $\hat{V}$. In the kicked pendulum case $\hat{T} = \hbar^2 \hat{L}^2/(2ml^2)$ and $\hat{V} = -mgl\cos\theta$, leading to:

$$\mathbf{U}(\tau, 0) = e^{ik\cos\theta} e^{-i\hat{L}^2 q} \ , \tag{2.26}$$

where the two dimensionless parameters k and q have the following form:

$$\begin{aligned} k &= \frac{ml^2\omega_0^2\tau}{\hbar} \\ q &= \frac{\hbar\tau}{2ml^2} \ . \end{aligned} \tag{2.27}$$

Notice that the product of k and q is a familiar object:

$$2kq = \omega_0^2\tau^2 = K \ , \tag{2.28}$$

i.e., the dimensionless kick-strength leading to chaos, in the classical case, when $K > K_c \approx 1$. Indeed, while $\hbar$ and the mass m explicitly appear in both k and q, they cancel in the product $2kq$. Interestingly, $k \propto m/\hbar$ while $q \propto \hbar/m$, which means that when m decreases q grows and quantum effects are likely more important, for a fixed value of $K = 2kq$; viceversa, when m increases classical physics should play a dominant role.

According to the Floquet analysis of the previous section, if $|\psi(0)\rangle$ denotes the initial state of the system, the state at time $t = n\tau^+$ (the $+$ reminds us that the δ-function has acted already) is simply:

$$|\psi(n\tau)\rangle = \hat{U}^n |\psi(0)\rangle \ . \tag{2.29}$$

As it turns out, a very convenient basis set in which to perform calculations, especially when the quantum kinetic term $\propto q$ is large, is that of angular momentum eigenstates $\hat{L}|m\rangle = m|m\rangle$ with m integers from $-\infty$ to $+\infty$:

$$\langle\theta|m\rangle = \frac{1}{\sqrt{2\pi}} e^{im\theta} \ . \tag{2.30}$$

Inserting identities in the form

$$\mathbb{1} = \sum_{m=-\infty}^{+\infty} |m\rangle\langle m| \ ,$$

we easily arrive at:

$$\psi_m^{(n)} = \sum_{m'=-\infty}^{+\infty} [\hat{U}^n]_{mm'} \ \psi_{m'}^{(0)} \ , \tag{2.31}$$

where $\psi_m^{(n)} = \langle m|\psi(n\tau)\rangle$, and $\psi_{m'}^{(0)} = \langle m'|\psi(0)\rangle$ are the wave-functions at time $t = n\tau$ and $t = 0$ in the angular momentum basis, and $[\hat{U}^n]_{mm'} = \langle m|\hat{U}^n|m'\rangle$. A very useful quantity to monitor is

$$P_n(m) = |\psi_m^{(n)}|^2 = \left| \sum_{m'=-\infty}^{+\infty} [\hat{U}^n]_{mm'} \psi_{m'}^{(0)} \right|^2 \ , \tag{2.32}$$

i.e., the probability of measuring a value of angular momentum equal to m at time $n\tau$, in terms of which the expectation value of $\hat{L}^2$, and hence of the total kinetic energy, at time $t = n\tau$ is expressed as:

$$\langle\hat{L}^2\rangle_n = \langle\psi(n\tau)|\hat{L}^2|\psi(n\tau)\rangle = \sum_{m=-\infty}^{+\infty} m^2 P_n(m) \ . \tag{2.33}$$

It is instructive to calculate the matrix $[\hat{U}]_{mm'}$:

$$[\hat{U}]_{mm'} = \langle m|e^{ik\cos\theta}e^{-i\hat{L}^2 q}|m'\rangle = e^{-iq(m')^2} i^{m-m'} J_{m-m'}(k) \,, \tag{2.34}$$

where we have made use of the Bessel identity:

$$\int_0^{2\pi} \frac{d\theta}{2\pi}\, e^{ik\cos\theta} e^{im\theta} = i^m J_m(k) \,. \tag{2.35}$$

By looking at the modulus of $|[\hat{U}]_{mm'}|^2 = J^2_{m-m'}(k)$, one easily discovers that this is peaked at values of $|m-m'| \sim k$, and decreases very fast when $|m-m'| \gg k$: the matrix $[\hat{U}]_{mm'}$ is therefore *banded*, with values decreasing very fast past a certain width $\sim k$ away from the main diagonal $m = m'$. Until now, we have used only the first part of the Floquet-theorem story: the fact that the evolution at any time can be written in terms of a $\mathbf{U}(\tau, 0)$.

To go a bit deeper into the struncture of the quantum probability $P_n(m)$, let us express $\hat{U}$ in terms of its eigenstates, the Floquet modes $|\phi_i(0)\rangle = |\phi_i\rangle$, and corresponding eigenphases $e^{-i\mu_i\tau}$:

$$\hat{U}(\tau, 0) = \sum_i e^{-i\mu_i\tau} |\phi_i\rangle\langle\phi_i| \,, \tag{2.36}$$

with $\mu_i\tau \in [-\pi, \pi]$. Since the different Floquet modes are orthogonal and normalized, we can immediately take the n-th power of $\hat{U}$:

$$\hat{U}^n = \sum_i e^{-in\mu_i\tau} |\phi_i\rangle\langle\phi_i| \,, \tag{2.37}$$

which is the great advantage of working with Floquet modes! Therefore, the matrix elements we need $[\hat{U}^n]_{mm'}$ are simply given by:

$$[\hat{U}^n]_{mm'} = \sum_i e^{-in\mu_i\tau} \langle m|\phi_i\rangle\langle\phi_i|m'\rangle = \sum_i e^{-in\mu_i\tau} [\Phi]_{mi}[\Phi^\dagger]_{im'} \,, \tag{2.38}$$

where we have defined $[\Phi]_{mi} = \langle m|\phi_i\rangle$ to be the matrix, in the angular momentum basis, containing the different Floquet modes as column vectors. Let us now go back to $P_n(m) = |\psi^{(n)}_m|^2$, and reexpress it as:

$$P_n(m) = |\psi^{(n)}_m|^2 = \left| \sum_i e^{-in\mu_i\tau} \sum_{m'} [\Phi]_{mi}[\Phi^\dagger]_{im'} \psi^{(0)}_{m'} \right|^2 \,. \tag{2.39}$$

Let us specialize our calculation to the important case where the initial state is the ground state of the kinetic energy term, i.e., is it all centered at $m = 0$: $\psi^{(0)}_m = \delta_{m,0}$ Then the sum over m' in Eq. 2.39 can be done easily, obtaining:

$$P_n(m) = \left| \sum_i e^{-in\mu_i\tau} [\Phi]_{mi}[\Phi^\dagger]_{i0} \right|^2 \,. \tag{2.40}$$

It is a simple matter to verify that, indeed, $P_{n=0}(m) = \delta_{m,0}$:

$$P_{n=0}(m) = \left| \sum_i [\Phi]_{mi}[\Phi^\dagger]_{i0} \right|^2 = \left| [\Phi\Phi^\dagger]_{m0} \right|^2 = \delta_{m,0} \,, \tag{2.41}$$

since $\Phi\Phi^\dagger = \mathbb{1}$.

The question now is what happens when the time n increases. Will the $P_n(m)$ keep brodening, in the classically chaotic region of parameters, as the (Brownian motion) classical diffusion would predict? We will see several surprises emerging! On general grounds, one might write the $|\sum_i z_i|^2$ appearing above as a double sum, on i and j, and then split the sum into one containing only diagonal ($i = j$) terms and one with off-diagonal ($i \neq j$) terms as follows:

$$\left|\sum_i z_i\right|^2 = \sum_{i,j} z_i z_j^* = \sum_i |z_i|^2 + \sum_{i\neq j} z_i z_j^* \,. \tag{2.42}$$

In some sense, you could call the off-diagonal contributions *interference terms*. [9] If we apply this simple idea to the expression in Eq. 2.40 we end up splitting it as follows:

$$P_n(m) = \underbrace{\sum_i \left|[\Phi]_{mi}[\Phi^\dagger]_{i0}\right|^2}_{P^{\rm Diag}(m)} + \underbrace{\sum_{i\neq j} e^{-in(\mu_i-\mu_j)\tau}[\Phi]_{mi}[\Phi^\dagger]_{i0}[\Phi]^*_{mj}[\Phi^\dagger]^*_{j0}}_{P_n^{\rm Interf}(m)} \,. \tag{2.43}$$

Notice that the time-index n completely disappears from the diagonal terms, i.e., $P^{\rm Diag}(m)$ does not depend on n, while it obviously survives in the interference part, indeed multipling the *difference* of Floquet quasi-energies in the phase-factor $e^{-in(\mu_i-\mu_j)\tau}$. This oscillating phase-factor, as you would guess, can lead to constructive or distructive interference effects. Let us see what happens for $m = 0$, for instance. Here you simply find that:

$$P^{\rm Diag}(m=0) = \sum_i \left|[\Phi]_{0i}[\Phi^\dagger]_{i0}\right|^2 = \sum_i \left||[\Phi]_{0i}|^2\right|^2 = \sum_i |[\Phi]_{0i}|^4 \leq 1 \,, \tag{2.44}$$

i.e., we have found what is known as *inverse participation ratio* (IPR): it gives information on roughly how many Floquet modes enter in the decomposition of the original $|m = 0\rangle$ states. So, in order to have $P_{n=0}(m) = \delta_{m,0}$ we need, for $n = 0$, a *constructive* interference contribution which increases $P^{\rm Diag}(m = 0) < 1$ to 1. For large time $n \to \infty$, however, the rapidly oscillating phase-factor $e^{-in(\mu_i-\mu_j)\tau}$ tend to cancel out the interference terms, with important exceptions, known as *quantum resonances*, which occur when the value of the parameter q measuring quantum fluctuations is a *rational* multiple of 2π: we will see this below in the particular case of $q = 2\pi$. When such resonances occur, the average $\langle \hat{L}^2 \rangle_n \sim n^2$, i.e., the quantum dynamics is *ballistic* rather than diffusive.

Summarizing, for values of q which are *irrational* multiples of 2π we expect that:

$$P_n(m) = P^{\rm Diag}(m) + P_n^{\rm Interf}(m) \overset{n\to\infty}{\longrightarrow} P^{\rm Diag}(m) \,, \tag{2.45}$$

which implies that the distribution does not broaden indefinitely, and the average kinetic energy *saturates* to a finite value. This saturation is often referred to as *Dynamical localization*.

[9] I mention here another simple n-independent bound that you can write by making use of the triangular inequality $|\sum_i z_i| \leq \sum_i |z_i|$. By applying it to the $P_n(m)$ in Eq. 2.40 you easily show that:

$$P_n(m) \leq \Big|\sum_i \Big|[\Phi]_{mi}[\Phi^\dagger]_{i0}\Big|\Big|^2 = P^{\rm bound}(m) \,.$$

One easily shows also that $P^{\rm bound}(m = 0) = 1$ but I have not been able to use it for other purposes.

The limit should be intended with some care: it is not an ordinary limit, since a lot of time-fluctuations generally persist. We will see in the next lecture its relationship with the more conventional Anderson localization for disordered one-dimensional tight-binding models. The resulting "limiting" distribution $P^{\rm Diag}(m)$, moreover, shows a behaviour that is clearly *non Gaussian*, but rather compatible with an exponentially localized "particle":

$$P^{\rm Diag}(m) \sim \frac{1}{l_s} e^{-2|m|/l_s} \ , \tag{2.46}$$

with a localization length l_s which appears to be connected with the classical diffusion constant D as $l_s = \alpha D$, with a numerical coefficient $\alpha \sim 1/2$.

Let us go back to the role of the parameter q multiplying the kinetic term. As mentioned above, only $K = 2kq$ enters in the classical dynamics, while q controls the quantum kinetic term. One can show that if q is a *rational multiple* of 2π funny things happen and the "particle" rather then localizing, moves in a ballistic way. I will now show this explicitly for $q = 2\pi$. The problem is best tackled directly in reals space θ. We can write:

$$\langle\theta|\hat{U}|\psi(0)\rangle\Big|_{q=2\pi} = e^{ik\cos\theta} e^{i2\pi\hat{L}^2} \psi^{(0)}(\theta) \ . \tag{2.47}$$

Since $\hat{L}^2$ can have only *integer* eigenvalues of the form m^2, it will give a phase factor $e^{i2\pi m^2} = 1$ and you can disregard it altogether, obtaining:

$$\langle\theta|\hat{U}|\psi(0)\rangle\Big|_{q=2\pi} = e^{ik\cos\theta} \psi^{(0)}(\theta) \ . \tag{2.48}$$

This implies that $\hat{U}$ is, for $q = 2\pi$, *diagonal* in the real space representation: $\langle\theta|\hat{U}|\theta'\rangle\Big|_{q=2\pi} = e^{ik\cos\theta}\delta(\theta - \theta')$. Therefore:

$$\psi^{(n)}(\theta) = \langle\theta|\hat{U}^n|\psi(0)\rangle\Big|_{q=2\pi} = e^{ink\cos\theta} \psi^{(0)}(\theta) \ , \tag{2.49}$$

a remarkable result which immediately implies (using integration by parts) that:

$$\begin{aligned} \langle\hat{L}^2\rangle_n = \int_0^{2\pi} \left|\frac{\partial}{\partial\theta}\psi^{(n)}(\theta)\right|^2 &\overset{q=2\pi}{=} \int_0^{2\pi} \left|e^{ik\cos\theta}\frac{\partial}{\partial\theta}\psi^{(0)}(\theta) - ink\sin\theta e^{ink\cos\theta}\psi^{(0)}(\theta)\right|^2 \\ &\overset{q=2\pi}{=} \langle\hat{L}^2\rangle_0 + n^2k^2 \int_0^{2\pi} \sin^2\theta \left|\psi^{(0)}(\theta)\right|^2 \ + \ O(n) \ , \end{aligned} \tag{2.50}$$

where you see a term increasing, *ballistically*, as n^2, and originating from the derivative of the phase-factor $e^{ikn\cos\theta}$. Similar phenomena occur for all q which are *rational* multiples of 2π. So, in order to see the "dynamical localization" you should in principle stay away from such q and consider only q which are *irrational* multiples of 2π.

Part III.

Introduction to Topological Insulators

3. Berry phase

I present in this chapter the essential properties of the so-called Berry phase [3] in quantum mechanics, concentrating on the crucial example of a spin-1/2 system. Traditional condensed matter applications, like the dynamical Jahn-Teller effect and other Born-Oppenheimer-related aspects are discussed in the literature — see, for instance, the very nice lecture notes by Raffaele Resta [4] — and will not be touched upon here. For references on the early experiments revealing the Berry phase, you can consult Ref. [5, Chap. 5].

3.1. Adiabatic theorem in quantum mechanics

I start with a statement of the adiabatic theorem, and a glimpse of the crucial ingredients in the proof. A full proof, quite heavy to digest, is given in the book by Messiah [6, p. 747].

Suppose the Hamiltonian depends on some external parameters $\mathbf{R}$, living in some n-dimensional space, which are changed in some prescribed manner along a path in parameter space $\mathbf{R}_s$, with $s \in [0,1]$, starting from $\mathbf{R}_0$ and ending in $\mathbf{R}_1$. We will assume that the parameters are changed very slowly, in a "suitably long" time T (see below for more details on the meaning of "long"), for instance by making a linear ramp of $s = t/T$, i.e., $\mathbf{R}(t) = \mathbf{R}_{t/T}$. [1]

Consider the instantaneous eigenstates $|\Phi_m(\mathbf{R})\rangle$ of the system for a given value of $\mathbf{R}$, assumed to be *non-degenerate*, [2] and the corresponding instantaneous eigenvalues $E_m(\mathbf{R})$. Clearly, they satisfy:

$$\widehat{H}(\mathbf{R})|\Phi_m(\mathbf{R})\rangle = E_m(\mathbf{R})|\Phi_m(\mathbf{R})\rangle \ . \tag{3.1}$$

Notice, however, that the overall phase in front of each $|\Phi_m(\mathbf{R})\rangle$ is rather arbitrary. Let us assume that an arbitrary choice of phases is made in such a way that $|\Phi_m(\mathbf{R})\rangle$ is continuous enough that we can take *derivatives* with respect to $\mathbf{R}$. [3] The problem we would like to study is the *time-dependent* Schrödinger equation

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = \widehat{H}(\mathbf{R}(t))|\Psi(t)\rangle \ , \tag{3.2}$$

with initial condition $|\Psi(0)\rangle = |\Phi_0(\mathbf{R}_0)\rangle$, i.e., starting from the instantaneous eigenstate $|\Phi_0\rangle$, which we arbitrarily labeled 0 (usually the ground state, but this is really not crucial)

[1] More general non-linear monotonic ramps can be considered as well.

[2] The generalization of the concept of Berry phase to a degenerate case has been studied by Wilczek and Zee [7].

[3] Indeed, any diagonalization routine would provide eigenstates with rather arbitrary phases. We will discuss some numerical aspects later on. We will also address the issue of defining smooth phases over all the manifold of the parameters, which can usually be done only *locally*.

at the initial value $\mathbf{R}_0$. It is useful to introduce right-away (they will be useful later on) the projector $\mathbb{P}(\mathbf{R}) = |\Phi_0(\mathbf{R})\rangle\langle\Phi_0(\mathbf{R})|$ and its orthogonal complement $\mathbb{Q}(\mathbf{R}) = \mathbb{1} - \mathbb{P}(\mathbf{R}) = \sum_{m\neq 0} |\Phi_m(\mathbf{R})\rangle\langle\Phi_m(\mathbf{R})|$. Changing variables from $t \in [0,T]$ to $s = t/T \in [0,1]$ we can equivalently re-express the time-dependent problem as:

$$i\hbar \frac{d}{ds} |\widetilde{\Psi}(s)\rangle = T\widehat{H}(\mathbf{R}_s)|\widetilde{\Psi}(s)\rangle \ , \tag{3.3}$$

where $|\widetilde{\Psi}(s)\rangle = |\Psi(t = sT)\rangle$. The statement of the adiabatic theorem is that if $E_0(\mathbf{R}_s)$ is *non-degenerate* and separated from all other eigenvalues $E_n(\mathbf{R}_s)$ by a *finite energy gap* $\hbar\omega_{n0}(s) = E_n(\mathbf{R}_s) - E_0(\mathbf{R}_s)$, then, for large enough T, the state essentially remains proportional to $|\Phi_0(\mathbf{R}_s)\rangle$, up to a phase-factor. [4]

To justify this result, start by writing the natural time-dependent *Ansatz* for $|\widetilde{\Psi}(s)\rangle$ based on the instantaneous eigenstates:

$$|\widetilde{\Psi}(s)\rangle = \sum_m C_m(s)\ \mathrm{e}^{-\frac{iT}{\hbar}\int_0^s ds' E_m(\mathbf{R}_{s'})}\ |\Phi_m(\mathbf{R}_s)\rangle \ , \tag{3.4}$$

where $C_m(0) = \delta_{m,0}$. For a more compact notation we will often shorten $E_m(s) = E_m(\mathbf{R}_s)$. The dynamical phase-factor $\mathrm{e}^{-\frac{iT}{\hbar}\int_0^s ds' E_m(s')}$ does its job in canceling, upon taking its s-derivative, against the right-hand-side $T\widehat{H}(\mathbf{R}_s)|\widetilde{\Psi}(s)\rangle$. The equations that the coefficients $C_m(s)$ have to satisfy are then given by:

$$\sum_m \mathrm{e}^{-\frac{iT}{\hbar}\int_0^s ds' E_m(s')} \left[\dot{C}_m(s)\ |\Phi_m(\mathbf{R}_s)\rangle + C_m(s)\ \dot{\mathbf{R}}_s \cdot |\boldsymbol{\nabla}_{\mathbf{R}}\Phi_m(\mathbf{R}_s)\rangle\right] = 0 \ , \tag{3.5}$$

where $\dot{C}_m$ and $\dot{\mathbf{R}}_s$ denote derivatives with respect to s, and we have explicitly used the fact that the states $|\Phi_m(\mathbf{R})\rangle$ are differentiable with respect to $\mathbf{R}$, i.e., the overall phase is chosen in a sufficiently smooth way. Taking now the scalar product with the state $|\Phi_n(\mathbf{R}_s)\rangle$ and rearranging terms we arrive at:

$$\dot{C}_n(s) = -\sum_m C_m(s)\ \mathrm{e}^{-\frac{iT}{\hbar}\int_0^s ds'(E_m - E_n)}\ \dot{\mathbf{R}}_s \cdot \langle\Phi_n(\mathbf{R}_s)|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_m(\mathbf{R}_s)\rangle \ . \tag{3.6}$$

Let us look more closely at the diagonal term appearing in the previous expression, which we can take out of the sum

$$\dot{C}_n(s) = -C_n(s)\ \underbrace{\dot{\mathbf{R}}_s \cdot \langle\Phi_n(\mathbf{R}_s)|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_n(\mathbf{R}_s)\rangle}_{-i\dot{\gamma}_n(s)} + \left(\sum_{m\neq n} \cdots\right) \tag{3.7}$$

where $\cdots$ indicates all the other terms with $m \neq n$. [5] Observe that the factor $\dot{\mathbf{R}}_s \cdot \langle\Phi_n(\mathbf{R}_s)|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_n(\mathbf{R}_s)\rangle$ is *purely imaginary*; more generally, $\langle\Phi_n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_n(\mathbf{R})\rangle$ is a purely

[4] If you define by $\widehat{U}_T(s)$ the evolution operator, satisfying

$$i\hbar \frac{d}{ds}\widehat{U}_T(s) = T\widehat{H}(\mathbf{R}_s)\ \widehat{U}_T(s) \ ,$$

with $\widehat{U}_T(0) = \mathbb{1}$, then a mathematically more precise statement of the adiabatic theorem is that:

$$\lim_{T\to\infty} \widehat{U}_T(s)\ \mathbb{P}(\mathbf{R}_0) = \mathbb{P}(\mathbf{R}_s) \lim_{T\to\infty} \widehat{U}_T(s) \ .$$

[5] In the following, we will show that these off-diagonal terms go to zero at least as $1/T$ for large T, due to rapidly oscillating phase factors $\mathrm{e}^{-\frac{iT}{\hbar}\int_0^s ds'(E_m - E_n)}$. This is, in some way, the essence of the adiabatic theorem.

imaginary vector, due to the normalization condition. Indeed, if you consider its real part you get:

$$\langle \Phi_n | \boldsymbol{\nabla}_{\mathbf{R}} \Phi_n \rangle + \langle \boldsymbol{\nabla}_{\mathbf{R}} \Phi_n | \Phi_n \rangle = \boldsymbol{\nabla}_{\mathbf{R}} \langle \Phi_n | \Phi_n \rangle = 0 \; .$$

Therefore, if you define

$$\gamma_n(s) \stackrel{def}{=} i \int_0^s ds' \; \dot{\mathbf{R}}_{s'} \cdot \langle \Phi_n(\mathbf{R}_{s'}) | \boldsymbol{\nabla}_{\mathbf{R}} \Phi_n(\mathbf{R}_{s'}) \rangle \; , \tag{3.8}$$

the quantity γ_n is automatically *real* and

$$\dot{C}_n(s) = i\dot{\gamma}_n(s) C_n(s) \; + \left(\sum_{m \neq n} \cdots \right) \; . \tag{3.9}$$

Let us pause for a moment to discuss the very important quantity γ_n. It is evident that γ_n is a line-integral along the path from $\mathbf{R}_0$ to $\mathbf{R}_s$ of the real vector field $i\langle \Phi_n(\mathbf{R}) | \boldsymbol{\nabla}_{\mathbf{R}} \Phi_n(\mathbf{R}) \rangle$, a field which, however, depends on the arbitrary (smooth) choice we made about the phases of the instantaneous eigenstates $|\Phi_n(\mathbf{R})\rangle$. As such, the quantity γ_n is *gauge dependent*, synonymous in the present context of the arbitrariness in the phase of $|\Phi_n(\mathbf{R})\rangle$. We will see how things change completely if we consider a *closed path* in parameter space with $\mathbf{R}_1 = \mathbf{R}_0$. Then the quantity $\gamma_n(1)$ will turn out to be *independent on the choice of phases* for the $|\Phi_n(\mathbf{R})\rangle$. [6] We shall return to this important quantity in the following. For the time-being, let us proceed with our adiabatic theorem "sketch of proof".

The previous considerations suggest that we can take off a further phase-factor from the coefficient $C_n(s)$ by writing $C_n(s) = \mathrm{e}^{i\gamma_n(s)} c_n(s)$. If we do that, the diagonal term cancels exactly and we are left with the following system of differential equations:

$$\dot{c}_n(s) = \sum_{m \neq n} \mathrm{e}^{\frac{iT}{\hbar} \int_0^s ds' (E_n - E_m)} \; F_{nm}(s) \; c_m(s) \; , \tag{3.10}$$

where the coefficients $F_{nm}(s)$ are given by:

$$F_{nm}(s) = -\mathrm{e}^{i[\gamma_m(s) - \gamma_n(s)]} \; \dot{\mathbf{R}}_s \cdot \langle \Phi_n(\mathbf{R}_s) | \boldsymbol{\nabla}_{\mathbf{R}} \Phi_m(\mathbf{R}_s) \rangle \; . \tag{3.11}$$

Upon integrating from 0 to s we get a system of integral equations:

$$c_n(s) = \delta_{n,0} + \sum_{m \neq n} \int_0^s ds' \; \mathrm{e}^{\frac{iT}{\hbar} \int_0^{s'} ds'' (E_n - E_m)} \; F_{nm}(s') \; c_m(s') \; ,$$

where we used the initial condition, $c_n(0) = \delta_{n,0}$. Consider now $n \neq 0$. The most important contribution originating from the sum on the right-hand-side is expected to come from the

[6] I should stress that the fact that an extra phase factor has to be included in such a way that $|\Psi_n(t)\rangle = \mathrm{e}^{i\gamma_n(t)} |\Phi_n(t)\rangle$, whatever smooth choice of phase is made for $|\Phi_n\rangle$, is *orthogonal* to its own time-derivative:

$$\langle \Psi_n(t) | \frac{d}{dt} \Psi_n(t) \rangle = 0 \; ,$$

as you can immediately verify, was well clear to many, long before Berry's paper, see for instance Messiah [6, footnote on p. 754] or Thouless [8, comment below Eq. 2.3]. The importance of Berry's contribution was to understand the deep meaning of this extra phase in certain circumstances.

term with $m = 0$, because c_0 starts from 1 at $s = 0$. [7] Therefore:

$$c_n(s) = \int_0^s ds' \, \mathrm{e}^{\frac{iT}{\hbar}\int_0^{s'} ds''(E_n - E_0)} F_{n0}(s') \, c_0(s') \; + \left(\sum_{m \neq (n,0)} \cdots \right) . \tag{3.12}$$

Let us examine in detail $F_{n0}(s)$:

$$F_{n0}(s) = -\mathrm{e}^{i[\gamma_0(s) - \gamma_n(s)]} \, \dot{\mathbf{R}}_s \cdot \langle \Phi_n(\mathbf{R}_s) | \boldsymbol{\nabla}_{\mathbf{R}} \Phi_0(\mathbf{R}_s) \rangle \, .$$

The crucial assumption in the statement of the adiabatic theorem is that the energy gap $\hbar\omega_{n0}(s) = E_n(s) - E_0(s)$ is never zero along the whole path. In other words, the eigenvalue E_0 is assumed to be *non-degenerate* and separated by a finite gap from all other states. Then, by taking the derivative of the time-independent Schrödinger problem in Eq. (3.1), and taking the scalar product with $\langle \Phi_n |$, it is immediate to prove that:

$$\langle \Phi_n(\mathbf{R}_s) | \boldsymbol{\nabla}_{\mathbf{R}} \Phi_0(\mathbf{R}_s) \rangle = - \frac{\langle \Phi_n(\mathbf{R}_s) | \boldsymbol{\nabla}_{\mathbf{R}} \widehat{H} | \Phi_0(\mathbf{R}_s) \rangle}{E_n(\mathbf{R}_s) - E_0(\mathbf{R}_s)} \, , \tag{3.13}$$

which, upon substitution in F_{n0} gives:

$$F_{n0}(s) = \mathrm{e}^{i[\gamma_0(s) - \gamma_n(s)]} \, \frac{\dot{\mathbf{R}}_s \cdot \langle \Phi_n(\mathbf{R}_s) | \boldsymbol{\nabla}_{\mathbf{R}} \widehat{H} | \Phi_0(\mathbf{R}_s) \rangle}{E_n(\mathbf{R}_s) - E_0(\mathbf{R}_s)} \, . \tag{3.14}$$

So, the larger (in modulus) is the gap $\hbar\omega_{n0} = E_n - E_0$, the smaller is F_{n0}. But this is not all. Integrating by parts the phase-factor in Eq. (3.12) brings down a factor $T\omega_{n0}$ in the denominator: [8]

$$c_n(s) = \frac{\mathrm{e}^{iT\int_0^{s'} ds'' \omega_{n0}}}{iT\omega_{n0}(s')} F_{n0}(s') \, c_0(s') \Big|_0^s - \int_0^s ds' \, \frac{\mathrm{e}^{iT\int_0^{s'} ds'' \omega_{n0}}}{iT\omega_{n0}(s')} \frac{d}{ds} \left(F_{n0}(s') \, c_0(s') \right) \cdots + \left(\sum_{m \neq (n,0)} \cdots \right) ,$$

showing that the coefficients $c_{n\neq 0}$ have an overall factor $1/T$ in front. One might be tempted to even put down a *condition for adiabaticity* by requiring the smallness of the first term, [9] i.e., for all $s \in [0, 1]$:

$$\left| \frac{F_{n0}(s)}{T\omega_{n0}(s)} \right| = \left| \frac{\hbar}{T} \, \frac{\dot{\mathbf{R}}_s \cdot \langle \Phi_n(\mathbf{R}_s) | \boldsymbol{\nabla}_{\mathbf{R}} \widehat{H} | \Phi_0(\mathbf{R}_s) \rangle}{[E_n(\mathbf{R}_s) - E_0(\mathbf{R}_s)]^2} \right| \ll 1 \, . \tag{3.15}$$

The procedure outlined above is a possible starting point for an *adiabatic perturbation theory* [6, p. 752], which we will later on explain in more detail and use to derive, following Thouless, an expression for the Hall conductivity of a two-dimensional insulator.

[7] One should be very careful in thinking that what we are giving is a "proof": indeed, there is an infinity of contributions with $m \neq (n, 0)$ and it is not clear that you can actually neglect them so easily. We stress it again: this is only a "gist" of the proof.

[8] In integrating by parts, we neglect and collect under the $\cdots$ a term coming from the derivative of the denominator $iT\omega_{n0}(s)$.

[9] Somewhat surprisingly, a lot of controversies have appeared in the recent literature about the nature of such a condition (i.e., its being sufficient, or necessary, or both, or neither). These controversies were initiated by a PRL by Marzlin and Sanders in 2004 [9]: look at the literature quoting this paper, for instance [10], if you are curious about this issue.

Summarizing: Whenever the eigenvalue $E_0(\mathbf{R}(t))$ is non-degenerate and well separated from all the other eigenvalues $E_n(\mathbf{R}(t))$ by a finite gap $\hbar\omega_{n0}$, the Schrödinger dynamics approximately "conserves the eigenstate manifold" $|\Phi_0(\mathbf{R})\rangle$. That is, in the limit of a sufficiently long time T employed in going from $\mathbf{R}_0$ to $\mathbf{R}_1$, one can disregard the possibility that the system gets excited into different states $|\Phi_n\rangle$, and the approximate state of the system, if the evolution starts from $|\Phi_0(\mathbf{R}_0)\rangle$, is given by (switching for convenience from s to t):

$$|\Psi(t)\rangle \approx \mathrm{e}^{i\gamma_0(t)}\ \mathrm{e}^{-\frac{i}{\hbar}\int_0^t dt' E_0(\mathbf{R}(t'))}\ |\Phi_0(\mathbf{R}(t))\rangle\ , \tag{3.16}$$

where the non-trivial extra phase you have to include is given by:

$$\gamma_0(t) \stackrel{def}{=} i\int_0^t dt'\ \dot{\mathbf{R}}(t')\cdot\langle\Phi_0(\mathbf{R}(t'))|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R}(t'))\rangle\ . \tag{3.17}$$

The fact that this extra phase is *geometrical* in nature can be seen, mathematically, from the property that $\gamma_0(T)$ is invariant by re-parametrization of the curve $\mathbf{R}(t)$: for instance if $t = sT$, then a factor T appears from the Jacobian $dt = Tds$ but is exactly canceled by a factor $1/T$ given by the derivative $\dot{\mathbf{R}}(t) = \frac{1}{T}\dot{\mathbf{R}}_s$. [10] Physically, you see that $\gamma_0(T)$ has a strict mechanical analogy in the *total work* done by the force field

$$\boldsymbol{\mathcal{A}}(\mathbf{R}) = i\langle\Phi_0(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R})\rangle = -\mathrm{Im}\langle\Phi_0(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R})\rangle\ , \tag{3.18}$$

in going from $\mathbf{R}_0$ to $\mathbf{R}_1$ along the path $\mathbf{R}(t)$: as such, the "work" depends in general on the path, but not on the "velocity" with which you travel in it. The second important property of the geometrical phase $\gamma_0(t)$ is that it *depends* on the choice of phase (assumed differentiable) we made for the eigenstate $|\Phi_0(\mathbf{R})\rangle$, except when we make a closed path in parameter space, i.e., $\mathbf{R}(T) = \mathbf{R}(0)$. We will see this in detail in the next section, where we will show that the "force field" introduced above — the so-called *Berry connection* $\boldsymbol{\mathcal{A}}(\mathbf{R})$ — changes as $\boldsymbol{\mathcal{A}} \to \boldsymbol{\mathcal{A}}' = \boldsymbol{\mathcal{A}} + \nabla\Lambda(\mathbf{R})$ when a smooth change of phase $|\Phi_0(\mathbf{R})\rangle \to |\Phi_0'(\mathbf{R})\rangle = \mathrm{e}^{-i\Lambda(\mathbf{R})}|\Phi_0(\mathbf{R})\rangle$ is performed.

If you assume adiabaticity, i.e., that the state evolves by always staying in the Φ_0-manifold, it is a simple matter to show that the geometric phase $\gamma_0(t)$ *has to be included* in order to satisfy the Schrödinger equation. Such a statement can be given a precise formulation, as shown in the following exercise. [11]

[10] More generally, you can easily prove that the same is true for any monotonic change of variables $t = g(s)$ where the function $g(s)$ is such that $g(0) = 0$ and $g(1) = T$.

[11] A note on the idea of *parallel transport*, often introduced in the present context. Let us define a new Hamiltonian $\mathcal{H}_0(\mathbf{R}) = \widehat{H}(\mathbf{R}) - E_0(\mathbf{R})\mathbb{1}$, which has the same eigenstates as $\widehat{H}$, and eigenvalues shifted in such a way that $|\Phi_0(\mathbf{R})\rangle$ is now an eigenstate of $\widehat{\mathcal{H}}_0(\mathbf{R})$ with 0 eigenvalue, i.e., $\widehat{\mathcal{H}}_0(\mathbf{R})|\Phi_0(\mathbf{R})\rangle = 0$. Then, as the exercise guides you to do, searching for the state $|\Psi(t)\rangle = \mathrm{e}^{i\lambda(t)}|\Phi_0(\mathbf{R}(t))\rangle$, that satisfies on average the Schrödinger equation

$$\langle\Psi(t)|\left(i\hbar\frac{d}{dt} - \widehat{\mathcal{H}}_0(\mathbf{R}(t))\right)|\Psi(t)\rangle = 0 \qquad \Longrightarrow \qquad i\hbar\langle\Psi(t)|\frac{d}{dt}\Psi(t)\rangle = 0\ ,$$

since $\langle\Psi(t)|\widehat{\mathcal{H}}_0(\mathbf{R}(t))|\Psi(t)\rangle = 0$. Now, normalization of $|\Psi(t)\rangle$ implies

$$\frac{d}{dt}\langle\Psi(t)|\Psi(t)\rangle = \langle\frac{d}{dt}\Psi(t)|\Psi(t)\rangle + \langle\Psi(t)|\frac{d}{dt}\Psi(t)\rangle = 2\mathrm{Re}\langle\Psi(t)|\frac{d}{dt}\Psi(t)\rangle = 0\ .$$

Solving the Schrödinger equation with the correct phase $\lambda(t)$, which is now purely geometrical, since the dynamical part due to E_0 has been explicitly dropped out, is therefore equivalent to finding the correct

Exercise 3.1. *Impose that:*

$$\langle\Psi(t)|\left(i\hbar\frac{d}{dt}-\widehat{H}(\mathbf{R}(t))\right)|\Psi(t)\rangle=0$$

where $|\Psi(t)\rangle = e^{i\lambda(t)}|\Phi_0(\mathbf{R}(t))\rangle$*, and verify that the phase* $\lambda(t)$ *you have to include is precisely given by the dynamical phase supplemented by the geometrical phase* $\gamma_0(t)$*, i.e.,*

$$\lambda(t)=\gamma_0(t)-\frac{1}{\hbar}\int_0^t dt' E_0(\mathbf{R}(t'))\ .$$

Let me end this section with a brief comment on adiabaticity for an *extensive* many body system, with an exponentially large number of states. In such a case you should not expect that adiabaticity can be strictly satisfied, even in presence of a gap, in the thermodynamic limit. This is possibly exemplified by recent results on the quantum Ising model in one-dimension [11]. The reason behind this failure of adiabaticity, no matter how slowly you change your parameters, is, I believe, related to the fact that the true overlap $|\langle\Phi_0(\mathbf{R}(t))|\Psi(t)\rangle|^2$ almost invariably goes exponentially to 0, like $\mathrm{e}^{-\alpha L}$, in the limit of large sizes $L\to\infty$; in turn, this is possibly related to the presence of an *exponentially large* number of states $|\Phi_n(\mathbf{R}(t))\rangle$ with $n\neq 0$: you can think of making each coefficient c_n small, but the cumulative effect of an exponentially large number of them can be dangerous for adiabaticity.

3.2. Berry phase: generalities

Let us explore another route to get the geometrical phase we have found in the previous section. Consider the phase-difference between two (0-th) eigenstates at points $\mathbf{R}_{s_1}$ and $\mathbf{R}_{s_2}$:

$$\mathrm{e}^{-i\Delta\phi_{12}}=\frac{\langle\Phi_0(\mathbf{R}_{s_1})|\Phi_0(\mathbf{R}_{s_2})\rangle}{|\langle\Phi_0(\mathbf{R}_{s_1})|\Phi_0(\mathbf{R}_{s_2})\rangle|}\ .$$

It is clear that:

$$\Delta\phi_{1,2}=-\mathrm{Im}\log\langle\Phi_0(\mathbf{R}_{s_1})|\Phi_0(\mathbf{R}_{s_2})\rangle\ ,$$

does depend on the the arbitrary choice of phases for the eigenstates. However, consider, for instance, three states and calculate the change of phase in the *triangle* in parameter space connecting the states:

$$\Delta\phi_{1,2}+\Delta\phi_{2,3}+\Delta\phi_{3,1}=-\mathrm{Im}\log\langle\Phi_0(\mathbf{R}_{s_1})|\Phi_0(\mathbf{R}_{s_2})\rangle\langle\Phi_0(\mathbf{R}_{s_2})|\Phi_0(\mathbf{R}_{s_3})\rangle\langle\Phi_0(\mathbf{R}_{s_3})|\Phi_0(\mathbf{R}_{s_1})\rangle\ .$$

A moment reflection will lead you to conclude that this quantity is indeed *independent* on the choice of phase you make for the eigenstates, because each state appears *as a ket and as a bra* in the expression. More generally, imagine having a *closed polygonal path* in parameter

phase $\lambda(t)$ for which

$$\langle\Psi(t)|\frac{d}{dt}\Psi(t)\rangle=0\ ,$$

(i.e., not only the real part of it, but the whole thing is zero!) a condition that is often called of *parallel transport*. This prescription on the phase of the instantaneous states was indeed known and used *before* Berry's paper, see for instance Messiah's book [6, footnote on p. 754].

space with $s_j \in [0,1]$, $j = 0, \dots P$, such that $s_0 = 0$ and $s_P = 1$ with $\mathbf{R}_1 = \mathbf{R}_0$. Then the phase difference accumulated along the polygonal path:

$$\gamma^{(P)} = \sum_{j=0}^{P-1} \Delta\phi_{j,j+1} = -\mathrm{Im} \log \langle \Phi_0(\mathbf{R}_0)|\Phi_0(\mathbf{R}_{s_1})\rangle\langle \Phi_0(\mathbf{R}_{s_1})|\Phi_0(\mathbf{R}_{s_2})\rangle \cdots \langle \Phi_0(\mathbf{R}_{s_{P-1}})|\Phi_0(\mathbf{R}_0)\rangle \ ,$$

does not depend at all on the arbitrary choice of the phases of $\Phi_0(\mathbf{R})$, as long as the path is *closed*. Notice, that you do not even have to assume that the phase choice is smooth! It does not matter: the arbitrary phases cancel in the loop. If you further assume that the phase-choice is such that $|\Phi_0(\mathbf{R})\rangle$ is *differentiable*, then one can show that:

$$\begin{aligned} \Delta\phi_{j,j+1} &= -\mathrm{Im} \log \langle \Phi_0(\mathbf{R}_{s_j})|\Phi_0(\mathbf{R}_{s_{j+1}})\rangle \\ &= -\mathrm{Im} \log \left(1 + \langle \Phi_0(\mathbf{R}_{s_j})|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R}_{s_j})\rangle \cdot \Delta\mathbf{R} + \cdots\right) \\ &= i\langle \Phi_0(\mathbf{R}_{s_j})|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R}_{s_j})\rangle \cdot \Delta\mathbf{R} + \cdots \ , \end{aligned} \tag{3.19}$$

with $\Delta\mathbf{R} = \mathbf{R}_{s_{j+1}} - \mathbf{R}_{s_j}$, where we used that $\log(1+z) = z + \cdots$, and that $\mathrm{Im}\langle\Phi_0|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0\rangle$ can be replaced by $-i\langle\Phi_0|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0\rangle$ because the scalar product is purely imaginary, as discussed before. In the limit in which the number of intervals P goes to ∞, the Riemann sums turn into a closed line-integral:

$$\lim_{P\to\infty} \gamma^{(P)} = \gamma = \oint_C \boldsymbol{\mathcal{A}}(\mathbf{R}) \cdot d\mathbf{R}$$

where C denotes the closed path, and the so-called *Berry connection* $\boldsymbol{\mathcal{A}}$ is defined as:

$$\boldsymbol{\mathcal{A}}(\mathbf{R}) = i\langle \Phi_0(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R})\rangle = -\mathrm{Im}\langle \Phi_0(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R})\rangle \ . \tag{3.20}$$

The Berry connection $\boldsymbol{\mathcal{A}}$ depends on the (smooth) choice of phases we make on $|\Phi_0(\mathbf{R})\rangle$. Suppose indeed we consider a new $|\Phi_0'(\mathbf{R})\rangle = \mathrm{e}^{-i\Lambda(\mathbf{R})}|\Phi_0(\mathbf{R})\rangle$. Then the associated Berry connection $\boldsymbol{\mathcal{A}}'$ is given by

$$\boldsymbol{\mathcal{A}}' = \boldsymbol{\mathcal{A}} + \boldsymbol{\nabla}_{\mathbf{R}}\Lambda(\mathbf{R}) \ , \tag{3.21}$$

i.e., a form identical to the change of gauge for the standard vector potential in electromagnetism. Obviously, Λ is irrelevant when we integrate $\boldsymbol{\mathcal{A}}$ over a *closed loop* C, and therefore the *closed-path Berry phase* γ is *gauge invariant!* As such, you expect γ to be *experimentally measurable*, through interferometric and spin-polarization-type experiments, as indeed was verified [5, Chap. 5].

The vector field (or 1-form) $\boldsymbol{\mathcal{A}}$ can related, by Stokes' theorem, to another important quantity: the analogue of the magnetic field $\mathbf{B}$. Suppose, indeed, that the parameter space in which $\mathbf{R}$ leaves in dimension $n = 3$. Then, we can calculate the "curl of $\boldsymbol{\mathcal{A}}$" as:

$$\boldsymbol{\mathcal{F}}(\mathbf{R}) = \boldsymbol{\nabla}_{\mathbf{R}} \times \boldsymbol{\mathcal{A}}(\mathbf{R}) = -\mathrm{Im}\langle \boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R})| \times |\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R})\rangle \ , \tag{3.22}$$

where we used the fact that $\boldsymbol{\nabla}_{\mathbf{R}} \times |\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0\rangle = 0$. Now, if the curve C is the boundary of some surface Σ (i.e., $C = \partial\Sigma$), then Stokes' theorem guarantees that:

$$\gamma = \oint_{\partial\Sigma} \boldsymbol{\mathcal{A}}(\mathbf{R}) \cdot d\mathbf{R} = \int_\Sigma \boldsymbol{\mathcal{F}}(\mathbf{R}) \cdot \mathbf{n} \ d\sigma \ . \tag{3.23}$$

In general dimension n, one cannot deal with the familiar "curl": one has to introduce the so-called 2-form to write Stokes theorem. Let us return to the expression in $d = 3$, where the curl works wonderfully well. The three components of $\boldsymbol{\mathcal{F}}(\mathbf{R})$ read:

$$\mathcal{F}_1(\mathbf{R}) = -\mathrm{Im}\Big[\langle\partial_2\Phi_0(\mathbf{R})|\partial_3\Phi_0(\mathbf{R})\rangle - \langle\partial_3\Phi_0(\mathbf{R})|\partial_2\Phi_0(\mathbf{R})\rangle\Big] \,, \tag{3.24}$$

and similar equations for $\mathcal{F}_2$ and $\mathcal{F}_3$ in the usual cyclic way. For a more compact notation we have indicated, as we will do from now on, $\partial_\alpha = \frac{\partial}{\partial R_\alpha}$. Notice that the Im-part is totally irrelevant, because the expression in parenthesis is *manifestly anti-symmetric*, and hence its Re-part vanishes by construction. Therefore we can equivalently write:

$$\mathcal{F}_1(\mathbf{R}) = i\Big[\langle\partial_2\Phi_0(\mathbf{R})|\partial_3\Phi_0(\mathbf{R})\rangle - \langle\partial_3\Phi_0(\mathbf{R})|\partial_2\Phi_0(\mathbf{R})\rangle\Big] = -2\mathrm{Im}\langle\partial_2\Phi_0(\mathbf{R})|\partial_3\Phi_0(\mathbf{R})\rangle \,. \tag{3.25}$$

It is now evident that a manifestly anti-symmetric object of the same form, known as *Berry curvature*, can be written in any dimension by defining:

$$\mathcal{F}_{\alpha\beta}(\mathbf{R}) = -2\mathrm{Im}\langle\partial_\alpha\Phi_0(\mathbf{R})|\partial_\beta\Phi_0(\mathbf{R})\rangle = i\Big[\langle\partial_\alpha\Phi_0(\mathbf{R})|\partial_\beta\Phi_0(\mathbf{R})\rangle - \langle\partial_\beta\Phi_0(\mathbf{R})|\partial_\alpha\Phi_0(\mathbf{R})\rangle\Big] \,, \tag{3.26}$$

the only difference being that in general this object has more components, $n(n-1)/2$ for general $n > 1$. By construction $\mathcal{F}_{\alpha\beta} = -\mathcal{F}_{\beta\alpha}$, hence $\mathcal{F}_{\alpha\alpha} = 0$. [12] Recalling that $\langle\Phi_0(\mathbf{R})|\partial_\beta\Phi_0(\mathbf{R})\rangle$ is purely imaginary, it is evident that:

$$\mathrm{Im}\Big[\langle\partial_\alpha\Phi_0(\mathbf{R})|\Phi_0(\mathbf{R})\rangle\langle\Phi_0(\mathbf{R})|\partial_\beta\Phi_0(\mathbf{R})\rangle\Big] = 0 \,.$$

This shows that we can freely insert a projector $\mathbb{Q}(\mathbf{R}) = \mathbb{1} - |\Phi_0(\mathbf{R})\rangle\langle\Phi_0(\mathbf{R})|$ in the definition of $\mathcal{F}_{\alpha\beta}(\mathbf{R})$ as follows:

$$\mathcal{F}_{\alpha\beta}(\mathbf{R}) = -2\mathrm{Im}\langle\partial_\alpha\Phi_0(\mathbf{R})|\mathbb{Q}(\mathbf{R})|\partial_\beta\Phi_0(\mathbf{R})\rangle \,. \tag{3.27}$$

The advantage of this way of writing is the *manifest gauge-invariance* of such an object. Indeed, let us see what happens if you do a smooth change of phase (gauge, in the new language) to the state

$$|\Phi_0(\mathbf{R})\rangle \to |\Phi_0'(\mathbf{R})\rangle = \mathrm{e}^{-i\Lambda(\mathbf{R})}|\Phi_0(\mathbf{R})\rangle \,.$$

Then:

$$|\partial_\beta\Phi_0'(\mathbf{R})\rangle = -i\partial_\beta\Lambda\ \mathrm{e}^{-i\Lambda(\mathbf{R})}|\Phi_0(\mathbf{R})\rangle \ + \ \mathrm{e}^{-i\Lambda(\mathbf{R})}|\partial_\beta\Phi_0(\mathbf{R})\rangle \,.$$

This shows that the new derivative has an extra term proportional to $\partial_\beta\Lambda$, which, however, is along $|\Phi_0(\mathbf{R})\rangle$ and therefore cancels out exactly when meeting the projector $\mathbb{Q}(\mathbf{R})$. In other words, you can easily convince yourself that:

$$\mathcal{F}_{\alpha\beta} \to \mathcal{F}'_{\alpha\beta} = -2\mathrm{Im}\langle\partial_\alpha\Phi_0'(\mathbf{R})|\mathbb{Q}(\mathbf{R})|\partial_\beta\Phi_0'(\mathbf{R})\rangle = \mathcal{F}_{\alpha\beta} \,,$$

[12] In dimension $n = 3$, the new tensorial notation is related to the traditional curl notation by $\mathcal{F}_1 = \mathcal{F}_{23}$, $\mathcal{F}_2 = \mathcal{F}_{31} = -\mathcal{F}_{13}$, $\mathcal{F}_3 = \mathcal{F}_{12}$.

i.e., the Berry curvature is manifestly *gauge invariant*, a result that should not surprise you from the knowledge of electromagnetism, if you think that $\boldsymbol{\mathcal{F}}$ plays the role of a magnetic field. [13]

We are now in the position to write a further expression for $\mathcal{F}_{\alpha\beta}(\mathbf{R})$, perhaps mathematically less elegant, but still physically very useful. If you recall that discussion on the adiabatic theorem, see Eq. (3.13), you will remember that for all states with $E_n \neq E_0$ we have (in the new notation): [14]

$$\langle \Phi_n(\mathbf{R}) | \partial_\beta \Phi_0(\mathbf{R}) \rangle = \frac{\langle \Phi_n(\mathbf{R}) | \partial_\beta \widehat{H} | \Phi_0(\mathbf{R}) \rangle}{E_0(\mathbf{R}) - E_n(\mathbf{R})} \ . \tag{3.31}$$

But this restriction on $n \neq 0$ is precisely that imposed by the projector $\mathbb{Q}$, hence:

$$\begin{aligned} \mathcal{F}_{\alpha\beta}(\mathbf{R}) &= -2\mathrm{Im} \sum_{n\neq 0} \langle \partial_\alpha \Phi_0(\mathbf{R}) | \Phi_n(\mathbf{R}) \rangle \langle \Phi_n(\mathbf{R}) | \partial_\beta \Phi_0(\mathbf{R}) \rangle \\ &= -2\mathrm{Im} \sum_{n\neq 0} \frac{\langle \Phi_0(\mathbf{R}) | \partial_\alpha \widehat{H} | \Phi_n(\mathbf{R}) \rangle \langle \Phi_n(\mathbf{R}) | \partial_\beta \widehat{H} | \Phi_0(\mathbf{R}) \rangle}{[E_0(\mathbf{R}) - E_n(\mathbf{R})]^2} \ . \end{aligned} \tag{3.32}$$

This expression for $\mathcal{F}_{\alpha\beta}$, involving standard energy denominators, often appears in physical calculations and also reveals some interesting aspects related to singularities of $\mathcal{F}_{\alpha\beta}(\mathbf{R})$. In particular, on notices that $\mathcal{F}_{\alpha\beta}(\mathbf{R})$ is singular whenever the gap between E_n and E_0 closes at

[13] Indeed, you can easily see that the Im-part prescription played no role in this proof. If you define, more generally, the tensor

$$\mathcal{G}_{\alpha\beta}(\mathbf{R}) = \langle \partial_\alpha \Phi_0(\mathbf{R}) | \mathbb{Q}(\mathbf{R}) | \partial_\beta \Phi_0(\mathbf{R}) \rangle \ , \tag{3.28}$$

of which $\mathcal{F}_{\alpha\beta}$ is the Im-part (or, equivalently, the anti-symmetric part), then $\mathcal{G}_{\alpha\beta}(\mathbf{R})$ is manifestly gauge-invariant. We can show that the Re$\mathcal{G}$ (i.e., the symmetric part) is related to a metric tensor associated to the distance

$$D^2_{\mathbf{R}_1,\mathbf{R}_2} = 1 - |\langle \Phi_0(\mathbf{R}_1) | \Phi_0(\mathbf{R}_2) \rangle|^2 \ .$$

Moreover, one can show that $\mathcal{G}_{\alpha\beta}$ can be written fully in terms of projectors (the most manifestly gauge-invariant way of writing):

$$\mathcal{G}_{\alpha\beta}(\mathbf{R}) = \mathrm{Tr}\Big[(\partial_\alpha \mathbb{P}(\mathbf{R})) \mathbb{Q}(\mathbf{R}) (\partial_\beta \mathbb{P}(\mathbf{R})) \Big] \ .$$

See Ref. [4].

[14] Recall here the similarity with the results of first-order perturbation theory. If $\hat{H}(\lambda) = \hat{H}_0 + \lambda \hat{V}$, we know that, for a non-degenerate state $|\Phi_n(\lambda)\rangle$ we can write:

$$|\Phi_n(\lambda)\rangle = |\Phi_n(0)\rangle + \lambda \sum_{m\neq n} |\Phi_m(0)\rangle \frac{\langle \Phi_m(0) | \hat{V} | \Phi_n(0) \rangle}{E_n(0) - E_m(0)} + O(\lambda^2) \ . \tag{3.29}$$

From this expression, and the fact that $\partial_\lambda \hat{H}(\lambda) = \hat{V}$, you immediately deduce that, for $m \neq n$:

$$\langle \Phi_m(0) | \partial_\lambda \Phi_n(\lambda) \rangle \Big|_{\lambda=0} = \frac{\langle \Phi_m(0) | \partial_\lambda \hat{H}(\lambda) | \Phi_n(0) \rangle}{E_n(0) - E_m(0)} \Big|_{\lambda=0} \ , \tag{3.30}$$

which closely mimics the result given in the text. However, what you almost invariably *never* learn when studying first-order perturbation theory, is that there is an important contribution to the change of the state in the direction of $|\Phi_n(0)\rangle$ itself, i.e., $\langle \Phi_n(0) | \partial_\lambda \Phi_n(\lambda) \rangle \Big|_{\lambda=0}$, which, sometimes, should be accounted for. This term, for which the first-order formula cannot be applied because of the energy denominators, is exactly at the origin of the Berry phase.

some point $\mathbf{R}^*$, which might be away from your physical trajectory $\mathbf{R}(t)$, but will nevertheless have important physical implications.

3.3. Berry phase: A spin S in a magnetic field

Let us consider an important example which allows us to carry out explicit calculations. Consider a spin S subject to a magnetic field $\mathbf{B}(t)$ which varies slowly in time. We will in the end consider the case of a $S = 1/2$, but carry out first the calculations for a general S. The Hamiltonian is:

$$\widehat{H}(\mathbf{B}(t)) = -g\mu\widehat{\mathbf{S}} \cdot \mathbf{B}(t) \,, \tag{3.33}$$

where g is the gyromagnetic ratio and $\mu = q\hbar/(2Mc)$ the magnetic moment, q being the charge of the particle and M its mass. Notice that the spin operators $\widehat{\mathbf{S}}$ are in units of $\hbar$ which is now hidden inside μ. Evidently, here $\mathbf{B}(t)$ plays the role of $\mathbf{R}(t)$ in our previous discussion.

We first tackle this problem in a traditional way, as you find it, for instance, in Sakurai, by calculating directly the Berry curvature without much discussion about how precisely the phase of the eigenstates are selected. We select the eigenstates when the magnetic field is $\mathbf{B}(t)$ as the eigenstates of $\widehat{S}_{z'}$, where $\hat{z}'$ is in the direction of $\mathbf{B}(t)$, i.e., $\widehat{S}_{z'} = \widehat{\mathbf{S}}\cdot\hat{\mathbf{B}}$, and indicate them as $|\Phi_m(\mathbf{B})\rangle$, with $m = -S, \cdots, S$ rather than with the standard expression $|S, m(\mathbf{B})\rangle$. The energy of such states is $E_m(\mathbf{B}) = -g\mu Bm$ where $B = |\mathbf{B}|$. In the previous notation, we should also calculate $\partial_\alpha \widehat{H} = -g\mu\widehat{S}_\alpha$. Let us focus on a given eigenstate m (which we denoted with 0 in the general discussion) and calculate accordingly the associated Berry curvature:

$$\mathcal{F}^{(m)}_{\alpha\beta}(\mathbf{B}) = -2\mathrm{Im}\sum_{m'\neq m} \frac{\langle\Phi_m(\mathbf{B})|\widehat{S}_\alpha|\Phi_{m'}(\mathbf{B})\rangle\langle\Phi_{m'}(\mathbf{B})|\widehat{S}_\beta|\Phi_m(\mathbf{B})\rangle}{B^2[m-m']^2} \,, \tag{3.34}$$

where a factor $(g\mu)^2$ cancelled in the numerator against the squared energies in the denominator. It is clear that when either α or β is z', then the results is zero because $|m'\rangle$ are eigenstates of $\widehat{S}_{z'}$. Therefore, the only non-vanishing term is:

$$\mathcal{F}^{(m)}_{x'y'}(\mathbf{B}) = -2\mathrm{Im}\sum_{m'\neq m} \frac{\langle\Phi_m(\mathbf{B})|\widehat{S}_{x'}|\Phi_{m'}(\mathbf{B})\rangle\langle\Phi_{m'}(\mathbf{B})|\widehat{S}_{y'}|\Phi_m(\mathbf{B})\rangle}{B^2[m-m']^2} \,. \tag{3.35}$$

If you recall that $\widehat{S}_{x'} = (\widehat{S}_+ + \widehat{S}_-)/2$ and $\widehat{S}_{y'} = (\widehat{S}_+ - \widehat{S}_-)/(2i)$ and that $\langle\Phi_{m\pm1}|\widehat{S}_\pm|\Phi_m\rangle = \sqrt{S(S+1)-m(m\pm1)}$, it is easy to calculate that:

$$\mathcal{F}^{(m)}_{x'y'}(\mathbf{B}) = -\frac{m}{B^2} \,, \tag{3.36}$$

but remember that this choice of spin direction is related to the direction of $\mathbf{B}$. Returning to the usual definition of curl in $n = 3$ dimension we have, therefore, a $\boldsymbol{\mathcal{F}}$ which is in the radial direction $\mathbf{B}$ and proportional to $-m/B^2$:

$$\boldsymbol{\mathcal{F}}^{(m)}(\mathbf{B}) = -m\frac{\hat{\mathbf{B}}}{B^2} \,. \tag{3.37}$$

Evidently, the Berry curvature has a singularity at the degeneracy point $\mathbf{B}^* = \mathbf{0}$ where all $2S+1$ eigenvalues are degenerate. Stokes' theorem then gives:

$$\gamma_m(C) = \int_{\Sigma_C} \boldsymbol{\mathcal{F}}^{(m)}(\mathbf{B}) \cdot \mathbf{n}\, d\sigma = -m \int_{\Sigma_C} \frac{\hat{\mathbf{B}}}{B^2} \cdot \hat{\mathbf{B}}\, B^2\, d\Omega = -m\Omega(C)\,, \tag{3.38}$$

where $\Omega(C)$ is the solid angle subtended by the circuit C from the degeneracy point $\mathbf{B}^* = \mathbf{0}$.

3.4. Berry phase: A closer look at the spin-1/2 case

Let us consider in more detail the case $S = 1/2$ which occurs particularly often, for instance in the discussion of the Haldane model. The reason for doing that (after all, the previous calculation was made for general S) is that we will better appreciate some subtleties about the choice of phase of the eigenstates which were somehow hidden in the previous approach: Remember that we selected the eigenstates as those of $\widehat{\mathbf{S}} \cdot \mathbf{B}$ but we did not have to discuss what phases they had, since the Berry curvature was gauge-invariant: this time, we will address questions about phases and the form of the Berry connection $\boldsymbol{\mathcal{A}}$ in more detail.

So, let us take as Hamiltonian the typical one of a spin-1/2 electron in a magnetic field

$$\widehat{H}(\mathbf{R}(t)) = g\mu_B \widehat{\mathbf{S}} \cdot \mathbf{B}(t) = \mathbf{R}(t) \cdot \hat{\boldsymbol{\sigma}}\,, \tag{3.39}$$

where we have reabsorbed a $g\mu_B/2$ inside a general vectorial parameter $\mathbf{R}(t) = (g\mu_B/2)\mathbf{B}(t)$. Assume now $\mathbf{R}$ to be parameterized by the usual spherical coordinates: R, the "distance" from the origin, and two polar angles θ and ϕ. The two eigenstates of the spin in direction $\mathbf{R}$ can be chosen to be:

$$|\Phi_{+\frac{1}{2}}(\mathbf{R})\rangle_N = \begin{pmatrix} \cos\frac{\theta}{2} \\ \mathrm{e}^{i\phi}\sin\frac{\theta}{2} \end{pmatrix} \qquad |\Phi_{-\frac{1}{2}}(\mathbf{R})\rangle_N = \begin{pmatrix} \mathrm{e}^{-i\phi}\sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix}\,, \tag{3.40}$$

with corresponding energy $E_{\pm\frac{1}{2}} = \pm R$. Again $\mathbf{R}^* = \mathbf{0}$ is a degeneracy point. Notice that this choice of phase of the eigenstates is not the only one possible, hence our subscript N to indicate that this choice is well defined everywhere around the North pole ($\theta = 0$) but is singular exactly at the South pole $\theta = \pi$ because there $\sin(\pi/2) = 1$ but the term $\mathrm{e}^{\pm i\phi}$ is totally undetermined. We will see how this singularity reflects itself in the form of the Berry connection. An alternative choice of phase is obtained by multiplying by $\mathrm{e}^{\mp i\phi}$, giving:

$$|\Phi_{+\frac{1}{2}}(\mathbf{R})\rangle_S = \begin{pmatrix} \mathrm{e}^{-i\phi}\cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix} \qquad |\Phi_{-\frac{1}{2}}(\mathbf{R})\rangle_S = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\mathrm{e}^{i\phi}\cos\frac{\theta}{2} \end{pmatrix}\,, \tag{3.41}$$

which is now regular all around the South pole, but singular at the North pole ($\theta = 0$).

Let us first calculate the Berry connection of the states $|\Phi_{\pm\frac{1}{2}}\rangle_N$. Using spherical coordinates we have:

$$\boldsymbol{\mathcal{A}} = \mathcal{A}_R \widehat{\mathbf{R}} + \mathcal{A}_\theta \widehat{\boldsymbol{\theta}} + \mathcal{A}_\phi \widehat{\boldsymbol{\phi}}\,, \tag{3.42}$$

where we have introduced the standard unit vectors along the spherical coordinates, and then

calculate

$$\begin{aligned}
\mathcal{A}^{(N)}_{R,\pm} &= i\langle\Phi_{\pm\frac{1}{2}}|\partial_R\Phi_{\pm\frac{1}{2}}\rangle_N = 0 \\
\mathcal{A}^{(N)}_{\theta,\pm} &= \frac{1}{R}i\langle\Phi_{\pm\frac{1}{2}}|\partial_\theta\Phi_{\pm\frac{1}{2}}\rangle_N = 0 \\
\mathcal{A}^{(N)}_{\phi,\pm} &= \frac{1}{R\sin\theta}i\langle\Phi_{\pm\frac{1}{2}}|\partial_\phi\Phi_{\pm\frac{1}{2}}\rangle_N = \mp\frac{\sin^2\frac{\theta}{2}}{R\sin\theta} = \mp\frac{1-\cos\theta}{2R\sin\theta}\ ,
\end{aligned} \tag{3.43}$$

which as a clear vortex singularity at the South pole. In a similar fashion, we can calculate:

$$\begin{aligned}
\mathcal{A}^{(S)}_{R,\pm} &= i\langle\Phi_{\pm\frac{1}{2}}|\partial_R\Phi_{\pm\frac{1}{2}}\rangle_S = 0 \\
\mathcal{A}^{(S)}_{\theta,\pm} &= \frac{1}{R}i\langle\Phi_{\pm\frac{1}{2}}|\partial_\theta\Phi_{\pm\frac{1}{2}}\rangle_S = 0 \\
\mathcal{A}^{(S)}_{\phi,\pm} &= \frac{1}{R\sin\theta}i\langle\Phi_{\pm\frac{1}{2}}|\partial_\phi\Phi_{\pm\frac{1}{2}}\rangle_S = \pm\frac{\cos^2\frac{\theta}{2}}{R\sin\theta} = \pm\frac{1+\cos\theta}{2R\sin\theta}\ ,
\end{aligned} \tag{3.44}$$

with a vortex singularity at the North pole.

To get the Berry curvature $\boldsymbol{\mathcal{F}} = \nabla\times\boldsymbol{\mathcal{A}}$, we calculate the curl in spherical coordinates:

$$\boldsymbol{\mathcal{F}} = \frac{\widehat{\mathbf{R}}}{R\sin\theta}\left[\partial_\theta(\sin\theta\mathcal{A}_\phi) - \partial_\phi\mathcal{A}_\theta\right] + \frac{\widehat{\boldsymbol{\theta}}}{R}\left[\frac{1}{\sin\theta}\partial_\phi\mathcal{A}_R - \partial_R(R\mathcal{A}_\phi)\right] + \frac{\widehat{\boldsymbol{\phi}}}{R}\left[\partial_R(R\mathcal{A}_\theta) - \partial_\theta\mathcal{A}_R\right]\ .$$

This immediately gives:

$$\boldsymbol{\mathcal{F}}_\pm = \frac{\widehat{\mathbf{R}}}{R\sin\theta}\left[\partial_\theta\left(\mp\frac{1-\cos\theta}{2R}\right)\right] = \mp\frac{1}{2}\frac{\widehat{\mathbf{R}}}{R^2}\ , \tag{3.45}$$

which coincides with Eq. (3.37) for $m = \pm\frac{1}{2}$. This $\boldsymbol{\mathcal{F}}$ looks like the magnetic field generated by a magnetic *monopole* at the origin. One immediately realizes that the same result is obtained by calculating $\nabla\times\boldsymbol{\mathcal{A}}^{(S)}_\pm$. In other words, the Berry curvature, which is gauge invariant, is singular at the origin $\mathbf{R}^* = \mathbf{0}$ but otherwise regular everywhere else and totally independent of the choice of the phases of the wave-functions, while the Berry connection has to have a vortex singularity somewhere on the sphere, for instance at the North pole, or at the South pole, the position of the vortex singularity depending on the choice of the phases of the wave-functions.

Notice that this calculation provides an answer to the point raised long ago by Dirac regarding the quantization of electric charges if a magnetic monopole exists. Since this is, in itself, a piece of fundamental physics, which is, moreover, strongly related to our subject, let me recall it for you, in the version devised by T.T. Wu and C.N. Yang. If a magnetic monopole of strength e_M exists, i.e., $\nabla\cdot\mathbf{B} = 4\pi e_M\delta(\mathbf{R})$, then the magnetic field around it is given by

$$\mathbf{B} = e_M\frac{\hat{\mathbf{R}}}{R^2}\ ,$$

exactly as the electric field generated by a charge. Contrary to the electric field case, where we search for a potential V such that $\mathbf{E} = -\boldsymbol{\nabla}V$, it is impossible to find a regular-everywhere vector potential $\mathbf{A}$ such that $\mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A}$. [15] To be more precise, one cannot find a single $\mathbf{A}$

[15] The argument given in the book by Sakurai, Sec. 2.6, is not very convincing. It goes as follows: if such a regular $\mathbf{A}$ would exist, then automatically $\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\times\mathbf{A}) = 0$, so that by Gauss theorem the flux of magnetic field around a surface enclosing $\mathbf{R}^* = \mathbf{0}$ should vanish, contrary to the fact that such a flux is $4\pi e_M$ for the monopole we have postulated. The objection to this is that nobody really assures that the regularity of $\mathbf{A}$ would eliminate the possibility of a delta-function emerging at $\mathbf{R} = \mathbf{0}$ from $\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\times\mathbf{A}) = 0$.

which is regular everywhere, except possibly at the origin $\mathbf{R}^* = \mathbf{0}$, which gives $\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}$. The proof of this fact is very instructive and quite pertinent to our discussion. Consider a sphere S^2 of radius $R = 1$ enclosing the monopole, and denote by Σ_N and Σ_S the North and South hemisphere, having, as a common frontier, the equator C. Assume an orientation on S compatible with the application of Stokes' theorem to Σ_S, i.e., such that

$$\int_{\Sigma_N} \mathbf{B} \cdot \mathbf{n}\, d\sigma = \int_C \mathbf{A} \cdot d\mathbf{R} \, .$$

In a similar way, one can apply Stokes' theorem to calculate the flux of $\mathbf{B}$ through Σ_S, but one has to be careful in noting that C is now traveled in the *opposite* direction and therefore:

$$\int_{\Sigma_S} \mathbf{B} \cdot \mathbf{n}\, d\sigma = \int_{-C} \mathbf{A} \cdot d\mathbf{R} = -\int_C \mathbf{A} \cdot d\mathbf{R} \, .$$

Summing together the two fluxes we conclude that

$$\int_{S^2} \mathbf{B} \cdot \mathbf{n}\, d\sigma = \int_C \mathbf{A} \cdot d\mathbf{R} - \int_C \mathbf{A} \cdot d\mathbf{R} = 0 \, ,$$

contrary to the fact that the flux should be $4\pi e_M$.

Yet another way of appreciating the inescapable necessity of a singularity, physically more transparent. Consider a small circle C, of radius $R \sin\theta$, encircling the North pole of the sphere at an angle θ. The magnetic flux through the solid angle $2\pi(1-\cos\theta)$ enclosed by C is simply $\Phi(\theta) = e_M 2\pi(1-\cos\theta)$. We can obviously represent such a flux by the line integral of a vector potential $\mathbf{A}^{(N)}$ tangential to the circle C in such a way that:

$$A^{(N)}_\phi \, 2\pi R \sin\theta = \Phi(\theta) = e_M 2\pi(1-\cos\theta) \quad \Longrightarrow \quad A^{(N)}_\phi(\theta) = \frac{e_M}{R} \frac{(1-\cos\theta)}{\sin\theta} \, .$$

As the angle θ increases, the total flux enclosed steadily increases towards $\Phi(\pi) = 4\pi e_M$, while the total length of the circumference of C first increases, for $0 < \theta < \pi/2$, but then, once we pass the equator, steadily decreases to shrink towards 0 when we are around the South pole: the vector potential $A^{(N)}$ has to compensate for the shrinking to 0 of the path-length by a divergence of its strength around the South pole, in essence, a *vortex singularity*. The same argument can be used to show that, no matter what point you chose to construct the vector potential, you will find a vortex singularity at the *opposite* point on the sphere.

The two solutions we have found above for $\boldsymbol{\mathcal{A}}$ are exactly two possible choices of $\mathbf{A}$, one regular around the North pole (with a vortex at the South pole), and one regular around the South pole (with a vortex at the North pole), both giving the monopole field:

$$\begin{aligned} \mathbf{A}^{(N)} &= \frac{e_M}{R} \frac{1-\cos\theta}{\sin\theta} \, \widehat{\boldsymbol{\phi}} \\ \mathbf{A}^{(S)} &= -\frac{e_M}{R} \frac{1+\cos\theta}{R\sin\theta} \, \widehat{\boldsymbol{\phi}} \, . \end{aligned} \tag{3.46}$$

I plot them in Fig. 3.1. Observe that the two choices are related by a gauge transformation $\Lambda = 2e_M\phi$:

$$\mathbf{A}^{(N)} - \mathbf{A}^{(S)} = 2e_M \frac{1}{R\sin\theta} \, \widehat{\boldsymbol{\phi}} = \boldsymbol{\nabla}\Lambda = \boldsymbol{\nabla}(2e_M\phi) \, . \tag{3.47}$$

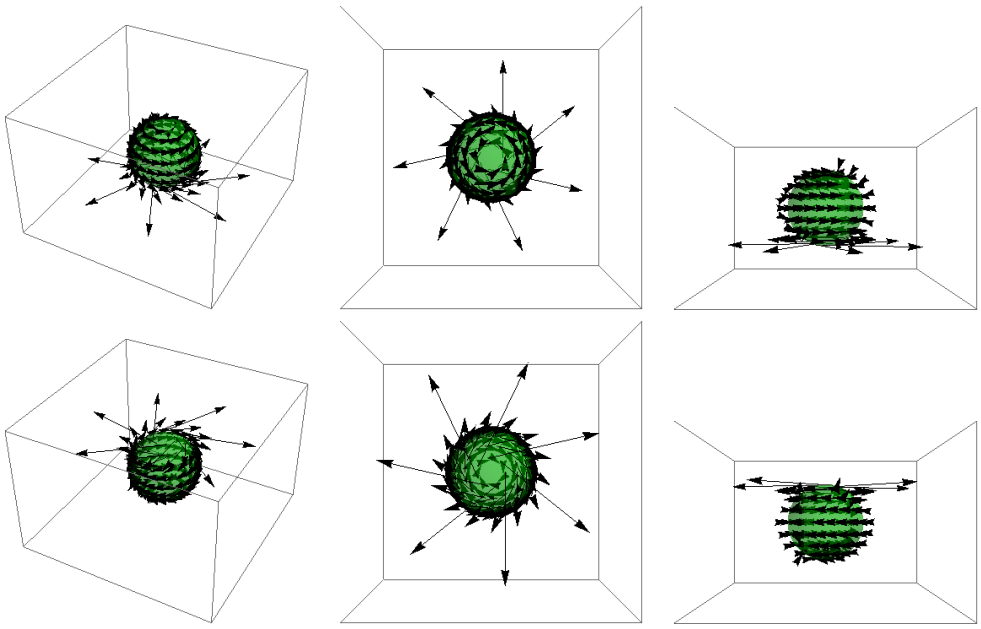

Figure 3.1.: Two of the possible choices of monopole vector potentials: $A^{(N)}$ (top, including a view from above and a front view) which is regular at the North pole and with a vortex at the south pole, and $A^{(S)}$ (bottom), vice-versa. Notice the opposite direction of rotation of the arrows in the two cases.

Consider next the orbital wave-function $\psi(\mathbf{R})$ of an electrically charged particle of charge e subject to the previous monopole field. As you know, the wave-function ψ must be single-valued everywhere, [16] but their phase depends on the choice of gauge. You can therefore write a $\psi^{(N)}$ and a $\psi^{(S)}$ which must be related by:

$$\psi^{(S)}(\mathbf{R}) = \exp\left(-i\frac{2ee_M}{\hbar c}\phi\right)\psi^{(N)}(\mathbf{R})\ . \tag{3.48}$$

Consider making a full turn by 2π, $\phi \to \phi + 2\pi$. Since both $\psi^{(N,S)}$ must be single-valued, then you immediately conclude that:

$$\frac{2ee_M}{\hbar c} = n \qquad \text{with } n = 0, \pm 1, \pm 2, \cdots \tag{3.49}$$

So, magnetic charges must be quantized in units of $\frac{\hbar c}{2|e|}$ and, vice-versa, if a magnetic monopole is assumed to exists, then all electric charges in the universe must be quantized in units of $\frac{\hbar c}{2|e_M|}$.

We stress that the previous discussion does *not* imply that quantum mechanics predicts the existence of magnetic monopoles. However, it unambiguously shows that a magnetic monopole, if ever found in nature, must be quantized in units of $\frac{\hbar c}{2e}$, where e is the electronic charge.

One last note which is of some relevance to the discussion of Chern insulators. Returning to the calculation of the flux of the $\mathbf{B}$ field through S^2, we can now amend our previous

[16] Recall that the wave-function is nothing but the amplitude in a position eigenkets expansion: there must be a unique amplitude associated to a given position ket, and a phase ambiguity is not possible.

calculation by saying that:

$$\begin{aligned}
\int_{\Sigma_N} \mathbf{B}\cdot\mathbf{n}\, d\sigma &= \int_C \mathbf{A}^{(N)}\cdot d\mathbf{R} \\
\int_{\Sigma_S} \mathbf{B}\cdot\mathbf{n}\, d\sigma &= -\int_C \mathbf{A}^{(S)}\cdot d\mathbf{R} \\
\int_{S^2} \mathbf{B}\cdot\mathbf{n}\, d\sigma &= \int_C [\mathbf{A}^{(N)}-\mathbf{A}^{(S)}]\cdot d\mathbf{R} = \int_C 2e_M \boldsymbol{\nabla}\phi\cdot d\mathbf{R} = 4\pi e_M \ . \qquad (3.50)
\end{aligned}$$

Notice that the line-integral of $\boldsymbol{\nabla}\phi$ around the equator C gives 2π, and not zero as one might be tempted to conclude: it gives 2π times the *winding number* of the angle ϕ appearing in the gauge transformation $\Lambda = 2e_M\phi$.

4. The Haldane model

4.1. Tight binding, magnetic fields, and currents

The full many-body problem for electrons in solids is quite formidable. Even neglecting the interaction between electrons and ionic vibrations (the so-called electron-phonon coupling terms), the Hamiltonian for the interacting electrons (in second quantization) would have the form:

$$\begin{aligned}\hat{H}_{\rm el} &= \sum_{\sigma} \int d\mathbf{x}\, \widehat{\Psi}^{\dagger}_{\sigma}(\mathbf{x}) \left[\frac{1}{2m} \left(-i\hbar \boldsymbol{\nabla} + \frac{e}{c}\mathbf{A} \right)^2 + v(\mathbf{x}) \right] \widehat{\Psi}_{\sigma}(\mathbf{x}) \\ &+ \sum_{\sigma,\sigma'} \frac{1}{2} \int d\mathbf{x} d\mathbf{x}'\, \widehat{\Psi}^{\dagger}_{\sigma'}(\mathbf{x}') \widehat{\Psi}^{\dagger}_{\sigma}(\mathbf{x}) \, \frac{e^2}{|\mathbf{x}-\mathbf{x}'|} \, \widehat{\Psi}_{\sigma}(\mathbf{x}) \widehat{\Psi}_{\sigma'}(\mathbf{x}') \, , \end{aligned} \tag{4.1}$$

where $\widehat{\Psi}_{\sigma}(\mathbf{x})$ is the second-quantization field operator, i.e., the operator that destroys a particle of spin σ at position $\mathbf{x}$, and the last Coulomb interaction term makes the problem essentially unsolvable. For future reference, we have included in the kinetic term a vector potential $\mathbf{A}$, describing an external electromagnetic field acting on the electrons. Possible scalar potential terms can be included in $v(\mathbf{x})$. Observe also that the kinetic energy term can be equivalently written in the more symmetric form: [1]

$$\hat{H}_{\rm kin} = \sum_{\sigma} \frac{1}{2m} \int d\mathbf{x} \left[\left(-i\hbar \boldsymbol{\nabla} + \frac{e}{c}\mathbf{A} \right) \widehat{\Psi}_{\sigma}(\mathbf{x}) \right]^{\dagger} \cdot \left[\left(-i\hbar \boldsymbol{\nabla} + \frac{e}{c}\mathbf{A} \right) \widehat{\Psi}_{\sigma}(\mathbf{x}) \right] , \tag{4.2}$$

where we see that the relevant operator is the ordinary momentum supplemented by the field term $(e/c)\mathbf{A}$ (related to the classical velocity times the mass):

$$\hat{\mathbf{\Pi}} = -i\hbar \boldsymbol{\nabla} + \frac{e}{c}\mathbf{A} \, . \tag{4.3}$$

One thing that is easy to derive, at this stage, is the form of the current density operator $\hat{\mathbf{j}}(\mathbf{x})$. One way to derive it, is to start from the density operator

$$\hat{n}(\mathbf{x}) = \sum_{\sigma} \widehat{\Psi}^{\dagger}_{\sigma}(\mathbf{x}) \widehat{\Psi}_{\sigma}(\mathbf{x}) \, , \tag{4.4}$$

and write down its Heisenberg's equation of motion in the form of a *continuity equation*:

$$\frac{d}{dt} \hat{n}_H(\mathbf{x},t) = \frac{1}{i\hbar} [\hat{n}_H(\mathbf{x},t), \hat{H}_{\rm el}] = -\boldsymbol{\nabla} \cdot \hat{\mathbf{j}}_H(\mathbf{x},t) \, .$$

[1] This forms manifestly shows that the kinetic energy is Hermitean and positive definite.

The final result has a form which is reminiscent of the familiar current density in ordinary quantum mechanics:

$$\hat{\mathbf{j}}(\mathbf{x}) = \frac{1}{2m}\sum_{\sigma}\left(\widehat{\Psi}^{\dagger}_{\sigma}(\mathbf{x})\Big[\hat{\mathbf{\Pi}}\widehat{\Psi}_{\sigma}(\mathbf{x})\Big] + \Big[\hat{\mathbf{\Pi}}\widehat{\Psi}_{\sigma}(\mathbf{x})\Big]^{\dagger}\widehat{\Psi}_{\sigma}(\mathbf{x})\right) , \tag{4.5}$$

while the electric current density has an extra factor $-e$: $\hat{\mathbf{j}}^{e}(\mathbf{x}) = -e\hat{\mathbf{j}}(\mathbf{x})$. [2] Notice that potential terms do not influence at all the current operator. Notice also that you can write the current operator as a functional derivative of the Hamiltonian with respect to $\mathbf{A}$:

$$\frac{\delta \hat{H}}{\delta \mathbf{A}(\mathbf{x})} = \frac{e}{c}\hat{\mathbf{j}}(\mathbf{x}) = -\frac{1}{c}\hat{\mathbf{j}}^{e}(\mathbf{x}) , \tag{4.7}$$

which in turns leads to the following way of writing the Hamiltonian:

$$\hat{H} = \hat{H}_{\mathbf{A}=0} - \frac{1}{c}\int d\mathbf{x}\, \hat{\mathbf{j}}^{e}(\mathbf{x})\cdot\mathbf{A}(\mathbf{x}) . \tag{4.8}$$

The field operators $\widehat{\Psi}_{\sigma}(\mathbf{x})$ can be expanded in any one-particle basis set of orbitals labeled by quantum numbers α, call them $\phi_{\alpha}(\mathbf{x})$, and associated destruction operators $\hat{c}_{\alpha\sigma}$, as:

$$\widehat{\Psi}_{\sigma}(\mathbf{x}) = \sum_{\alpha}\phi_{\alpha}(\mathbf{x})\,\hat{c}_{\alpha\sigma} . \tag{4.9}$$

There is a large freedom in the choice of the basis $\phi_{\alpha}(\mathbf{x})$. Consider, for the time being, a system in absence of vector potential, $\mathbf{A} = 0$, for simplicity. One could select plane-waves $\phi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}}e^{i\mathbf{k}\cdot\mathbf{r}}$, which are eigenstates of $\hat{\mathbf{p}}^2/2m$. The alternative choice of $\phi_{n\mathbf{k}}(\mathbf{x})$ as the Bloch states of the particle in the periodic potential $v_{\rm per}(\mathbf{x})$, where n is a band index and $\mathbf{k}$ a wave-vector running in the Brillouin Zone (BZ) of the reciprocal lattice, evidently diagonalizes the $\hat{\mathbf{p}}^2/2m + v_{\rm per}(\mathbf{x})$ part of the Hamiltonian. One could write an expression of $\hat{H}_{\rm el}$ in terms of such states, introducing destruction operators $\hat{c}_{n\mathbf{k}\sigma}$, but, without even doing the calculation you realize that the Coulomb *many-body* mixing of states is inevitable. There is no way around. To treat the Coulomb potential in a some fair way, one possibility is to use basis states (approximately) localized around each site. Technically, this is done by a transformation from Bloch states to *Wannier states*. Without going into details (see a Solid State textbook, if you are curious), we simply state that we can in principle form appropriate states $w_{n\mathbf{r}}(\mathbf{x})$, as many as there are bands (labeled by n), around each lattice site $\mathbf{r}$, and in terms of the corresponding $\hat{c}_{n\mathbf{r}\sigma}$ express in the usual way the Hamiltonian $\hat{H}_{\rm el}$. The full expression with all possible bands n is useless, in practice.

A particularly important approach in many-body theory is, however, the following: *single-out a few important bands* in the problem you want to treat, and *disregard all other bands* altogether. For the case of a *single band*, we label by $w_{\mathbf{r}}(\mathbf{x})$ the corresponding Wannier orbitals (neglecting any band index n), and by $\hat{c}_{\mathbf{r}\sigma}$ the corresponding destruction operators, and approximate the field operator as:

$$\widehat{\Psi}_{\sigma}(\mathbf{x}) \approx \sum_{\mathbf{r}} w_{\mathbf{r}}(\mathbf{x})\,\hat{c}_{\mathbf{r}\sigma} . \tag{4.10}$$

[2] You can make the $\mathbf{A}$ term explicit by writing:

$$\hat{\mathbf{j}}^{e}(\mathbf{x}) = -\frac{e}{2m}\sum_{\sigma}\left(\widehat{\Psi}^{\dagger}_{\sigma}(\mathbf{x})\Big[\hat{\mathbf{p}}\widehat{\Psi}_{\sigma}(\mathbf{x})\Big] + \Big[\hat{\mathbf{p}}\widehat{\Psi}_{\sigma}(\mathbf{x})\Big]^{\dagger}\widehat{\Psi}_{\sigma}(\mathbf{x})\right) - \frac{e^2}{mc}\mathbf{A}(\mathbf{x})\,\hat{n}(\mathbf{x}) . \tag{4.6}$$

In this rather drastically restricted basis set, setting for a while $\mathbf{A} = 0$, the Hamiltonian reads:

$$\hat{H}_{\rm el} = \underbrace{\sum_{\sigma}\sum_{\mathbf{r}\neq\mathbf{r}'} h_{\mathbf{r}',\mathbf{r}}\hat{c}^{\dagger}_{\mathbf{r}'\sigma}\hat{c}_{\mathbf{r}\sigma} \; + \; \sum_{\sigma}\sum_{\mathbf{r}} \epsilon_{\mathbf{r}}\hat{c}^{\dagger}_{\mathbf{r}\sigma}\hat{c}_{\mathbf{r}\sigma}}_{\hat{H}_0} \; + (\cdots) \; , \tag{4.11}$$

where $h_{\mathbf{r}',\mathbf{r}}$ represents the amplitude for the electron to hop, conserving its spin, from orbital $w_{\mathbf{r}}$ to some neighbor $w_{\mathbf{r}'}$ on the lattice, [3]

$$h_{\mathbf{r}',\mathbf{r}} = \int d\mathbf{x}\; w^{*}_{\mathbf{r}'}(\mathbf{x})\Big[\frac{\hat{\mathbf{p}}^2}{2m} + v(\mathbf{x})\Big] w_{\mathbf{r}}(\mathbf{x}) \; , \tag{4.12}$$

$\epsilon_{\mathbf{r}}$ is the diagonal ("atomic") energy of the orbital $w_{\mathbf{r}}$ at site $\mathbf{r}$, while $(\cdots)$ hides all the interaction-generated terms (see, for instance, a discussion of the Hubbard model physics), which we shall not discuss in the following.

How do we treat a magnetic field in a tight-binding scheme? One would be tempted to simply substitute $\hat{\mathbf{p}} \to \hat{\mathbf{\Pi}} = \hat{\mathbf{p}} + \frac{e}{c}\mathbf{A}$ in the previous expression for $h_{\mathbf{r}',\mathbf{r}}$, but that would not lead to a *gauge invariant* expression, and is therefore a *wrong* thing to do. It is not infinitely hard to get convinced that a reasonable gauge-invariant [4] way of introducing the vector potential is by modifying the hopping amplitudes according to the so-called *Peierls' substitution*:

$$h_{\mathbf{r}',\mathbf{r}} \to h^{\mathbf{A}}_{\mathbf{r}',\mathbf{r}} \equiv h_{\mathbf{r}',\mathbf{r}}\; \mathrm{e}^{-i\frac{e}{\hbar c}\int_{\mathbf{r}}^{\mathbf{r}'}\mathbf{A}\cdot d\mathbf{l}} \; , \tag{4.13}$$

where the line-integral is calculated on a *straight line* connecting $\mathbf{r}$ to $\mathbf{r}'$. Such a line-integral suggests that we can introduce an average vector potential living on the link $(\mathbf{r},\mathbf{r}')$ as follows:

$$\mathbf{A}_{\mathbf{r}',\mathbf{r}}\cdot(\mathbf{r}'-\mathbf{r}) \equiv \int_{\mathbf{r}}^{\mathbf{r}'}\mathbf{A}\cdot d\mathbf{l} \; , \tag{4.14}$$

where evidently $\mathbf{A}_{\mathbf{r}',\mathbf{r}} = \mathbf{A}_{\mathbf{r},\mathbf{r}'}$. For an elementary justification of the Peierls' substitution, see for instance Feynman's Lectures on Quantum Mechanics, Chapter 21. [5]

[3] The reversed process has to have amplitude $h_{\mathbf{r},\mathbf{r}'} = h^{*}_{\mathbf{r}',\mathbf{r}}$, in order for $\hat{H}$ to be Hermitean. Very often, one can make a choice of phases for the Bloch/Wannier orbitals such that $h_{\mathbf{r}',\mathbf{r}}$ is real, in absence of magnetic fields.

[4] If you change $\mathbf{A} \to \mathbf{A} + \boldsymbol{\nabla}\Lambda$ then the phase factors change as:

$$\mathrm{e}^{-i(e/\hbar c)\int_{\mathbf{r}'}^{\mathbf{r}}\mathbf{A}\cdot d\mathbf{l}} \to \mathrm{e}^{-i(e/\hbar c)\int_{\mathbf{r}'}^{\mathbf{r}}\mathbf{A}\cdot d\mathbf{l}}\mathrm{e}^{-i(e/\hbar c)(\Lambda_{\mathbf{r}}-\Lambda_{\mathbf{r}'})} \; ,$$

and you can easily get rid of these extra phase factors by a unitary transformation that changes $\hat{c}_{\mathbf{r}\sigma} \to \tilde{c}_{\mathbf{r}\sigma} = \hat{c}_{\mathbf{r}\sigma}\mathrm{e}^{-i(e/\hbar c)\Lambda_{\mathbf{r}}}$.

[5] Here is the essence of the argument, written in first quantization. Consider a single electron wave-function $\psi(\mathbf{r})$ in two dimensions, and discretize the Laplacian on a square grid of side a. Including the Peierls' substitution phases we have:

$$-t\sum_{\mathbf{r}'\in N(\mathbf{r})}\mathrm{e}^{-i(e/\hbar c)\int_{\mathbf{r}'}^{\mathbf{r}}\mathbf{A}\cdot d\mathbf{l}}\psi_{\mathbf{r}'} + [4t + v(\mathbf{r})]\psi_{\mathbf{r}} = E\psi_{\mathbf{r}} \; , \tag{4.15}$$

where $t = \hbar^2/(2ma^2)$ and $N(\mathbf{r})$ denotes the four neighbors of site $\mathbf{r}$ which we can also express as $\mathbf{r}' = \mathbf{r} + \boldsymbol{\delta}$ with $\boldsymbol{\delta} = \pm a\hat{\mathbf{x}}, \pm a\hat{\mathbf{y}}$. First notice that, for small a, we can calculate $\int_{\mathbf{r}'}^{\mathbf{r}}\mathbf{A}\cdot d\mathbf{l} = -\boldsymbol{\delta}\cdot\mathbf{A}(\mathbf{r})$, where $\boldsymbol{\delta} = \mathbf{r}' - \mathbf{r}$, and hence expand the phase factor as

$$\mathrm{e}^{-i(e/\hbar c)\int_{\mathbf{r}'}^{\mathbf{r}}\mathbf{A}\cdot d\mathbf{l}} \approx 1 + i\frac{e}{\hbar c}\boldsymbol{\delta}\cdot\mathbf{A} - \frac{1}{2}\frac{e^2}{\hbar^2 c^2}(\boldsymbol{\delta}\cdot\mathbf{A})^2 + \cdots$$

It remains to address the issue of how to construct a current density operator in the tight-binding approximation. Once again, the naïve approach of substituting $\widehat{\Psi}_\sigma(\mathbf{x}) \approx \sum_{\mathbf{r}} w_{\mathbf{r}}(\mathbf{x})\ \hat{c}_{\mathbf{r}\sigma}$ in the continuum expression for $\hat{\mathbf{j}}(\mathbf{x})$ is plagued by many problems. A sensible way of deriving a physically sound expression for the current starts again from the Heisenberg's equation of motion, this time written for the local density $\hat{n}_{\mathbf{r}} = \sum_\sigma \hat{c}^\dagger_{\mathbf{r}\sigma}\hat{c}_{\mathbf{r}\sigma}$. From the continuity equation for the density, [6] omitting to indicate the time-dependence of all Heisenberg operators, we have:

$$\frac{d}{dt}\hat{n}_{\mathbf{r}} = \frac{1}{i\hbar}[\hat{n}_{\mathbf{r}}, \hat{H}_0] = \frac{i}{\hbar}\sum_\sigma \sum_{\mathbf{r}'}^{\neq \mathbf{r}} \left(h^{\mathbf{A}}_{\mathbf{r}',\mathbf{r}} \hat{c}^\dagger_{\mathbf{r}'\sigma}\hat{c}_{\mathbf{r}\sigma} - h^{\mathbf{A}}_{\mathbf{r},\mathbf{r}'} \hat{c}^\dagger_{\mathbf{r}\sigma}\hat{c}_{\mathbf{r}'\sigma} \right) . \tag{4.16}$$

Here we have assumed for $\hat{H}_0$ only the "kinetic-energy" term of the Hamiltonian. [7] The right-hand side has to be interpreted as the lattice version of $-\boldsymbol{\nabla}\cdot\hat{\mathbf{j}}$. More precisely, we define the following current operator on each link from $\mathbf{r} \to \mathbf{r}'$ where $h^{\mathbf{A}}_{\mathbf{r}',\mathbf{r}} \neq 0$:

$$\hat{\mathbf{j}}_{\mathbf{r}',\mathbf{r}} = -\frac{i}{\hbar}(\mathbf{r}' - \mathbf{r}) \sum_\sigma \left[h^{\mathbf{A}}_{\mathbf{r}',\mathbf{r}} \hat{c}^\dagger_{\mathbf{r}'\sigma}\hat{c}_{\mathbf{r}\sigma} - H.c. \right] = \hat{\mathbf{j}}_{\mathbf{r},\mathbf{r}'} . \tag{4.17}$$

Then, denoting by $\mathbf{a} = \mathbf{r}' - \mathbf{r}$ the vectors connecting $\mathbf{r}$ to its tight-binding "neighbors", is clear that what the continuity equation in Eq. (4.16) is telling us can be rewritten as:

$$\frac{d}{dt}\hat{n}_{\mathbf{r}} = -\sum_{\mathbf{a}} \frac{1}{|\mathbf{a}|^2}\, \hat{\mathbf{j}}_{\mathbf{r}+\mathbf{a},\mathbf{r}} \cdot \mathbf{a} , \tag{4.18}$$

where the right-hand side, the lattice version of $-\boldsymbol{\nabla}\cdot\hat{\mathbf{j}}$, suggests a simple interpretation in terms of fluxes of current going through the surface normal to the unit vector $\mathbf{a}/|\mathbf{a}|$, and indeed reproduces the standard discretization of a divergence on a cubic lattice with nearest-neighbor couplings. The total current is given by the sum of the currents on all bonds, counted only once:

$$\widehat{\mathbf{J}} = \frac{1}{2}\sum_{\mathbf{r}}\sum_{\mathbf{a}} \hat{\mathbf{j}}_{\mathbf{r}+\mathbf{a},\mathbf{r}} . \tag{4.19}$$

Next, Taylor-expand up to second order $\psi(\mathbf{r}' = \mathbf{r} + \boldsymbol{\delta})$ as:

$$\psi_{\mathbf{r}'} = \psi_{\mathbf{r}} + \boldsymbol{\delta}\cdot\boldsymbol{\nabla}\psi_{\mathbf{r}} + \frac{1}{2}\sum_{\alpha,\beta}\delta_\alpha\delta_\beta\partial_\alpha\partial_\beta\psi_{\mathbf{r}} + \cdots .$$

Finally, put together these ingredients, in the calculation of

$$-t\sum_{\mathbf{r}'=\mathbf{r}+\boldsymbol{\delta}} \mathrm{e}^{-i(e/\hbar c)\int_{\mathbf{r}'}^{\mathbf{r}}\mathbf{A}\cdot d\mathbf{l}}\ \psi_{\mathbf{r}'} + 4t\psi_{\mathbf{r}} ,$$

collecting terms of different order in $\boldsymbol{\delta}$, taking due notice of the fact that $t = \hbar^2/(2ma^2)$ contains a factor a^2 in the denominator that must be cancelled for $a \to 0$ by the numerator. Indeed, the terms of order 0 are $-4t + 4t = 0$. The terms of order 1 in $\boldsymbol{\delta}$ are *odd* in $\boldsymbol{\delta}$ and therefore cancel when you take the $\sum_{\boldsymbol{\delta}}$. The terms of order 2 in $\boldsymbol{\delta}$ have a factor a^2 that cancels against the denominator of t and $\cdots$ *exactly the right terms expected*: $(1/2m)(\hat{\mathbf{p}} + (e/c)\mathbf{A})^2\psi$. This shows that, indeed, the tight-binding-like form with Peierls phases reproduces, for $a \to 0$, the correct continuum equation.

[6] In the derivation, one has to take the commutator of $[\hat{c}^\dagger_{\mathbf{r}\sigma}\hat{c}_{\mathbf{r}\sigma}, \hat{c}^\dagger_{\mathbf{r}''\sigma'}\hat{c}_{\mathbf{r}'\sigma'}]$, which proceeds by first using $[A, BC] = [A, B]C + B[A, C]$, and then using $\{AB, C\} = A\{B, C\} - \{A, C\}B$ to exploit the canonical commutation relations of fermions.

[7] Hubbard-like interaction terms, depending on density-density operators, would not change the result, but general interaction terms which do not commute with $\hat{n}_{\mathbf{r}}$ would give extra contributions. Moreover, one might be puzzled by the fact that, strictly speaking, the tight-binding kinetic term includes one-particle potential contributions as well, and is not of purely kinetic origin.

An alternative derivation of all these expressions should be possible by working in *momentum space*, where one can deal with continuous variables, and the divergence reads $\mathbf{q}\cdot\hat{\mathbf{j}}_{\mathbf{q}}$. A further alternative derivation uses the fact that the current operator should be a derivative of the Hamiltonian with respect to the vector potential, as in the continuum case of Eq. (4.7). From the Hamiltonian written in the tight-binding form Eq. (4.11), with the Peierls' substitution $h_{\mathbf{r}',\mathbf{r}} \to h^{\mathbf{A}}_{\mathbf{r}',\mathbf{r}}$, taking a partial derivative with respect to the link vector potential $\mathbf{A}_{\mathbf{r}',\mathbf{r}}$ introduced above, we easily establish that:

$$\frac{\partial \hat{H}}{\partial \mathbf{A}_{\mathbf{r}',\mathbf{r}}} = -\frac{ie}{\hbar c}(\mathbf{r}'-\mathbf{r})\sum_{\sigma}\left[h^{\mathbf{A}}_{\mathbf{r}',\mathbf{r}}\hat{c}^{\dagger}_{\mathbf{r}'\sigma}\hat{c}_{\mathbf{r}\sigma} - H.c.\right] = \frac{e}{c}\hat{\mathbf{j}}_{\mathbf{r},\mathbf{r}'} = -\frac{1}{c}\hat{\mathbf{j}}^{e}_{\mathbf{r},\mathbf{r}'}\,. \tag{4.20}$$

This is probably the easiest and most transparent derivation, once the Peierls' substitution is adopted.

4.2. The Haldane model

Consider now a graphene sheet (two-dimensional system) with atoms sitting at the sites of a honeycomb lattice (see Fig. 4.1), and a tight-binding electronic hopping Hamiltonian. Since the spin will play no role in the present discussion (although it will reappear soon,

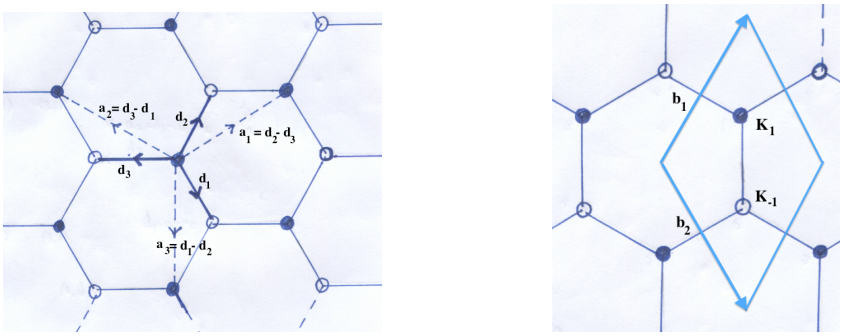

Figure 4.1.: The honeycomb lattice (left), and the associated reciprocal lattice with a possible choice of a rhombic Brillouin Zone (right).

when discussing the Kane-Mele model), we will ignore it from now on in the present chapter. The honeycomb lattice is made of two inter-penetrating Bravais triangular sublattices, which we denote by A and B. Starting from an A-site, the nearest-neighbor sites are B-type and they are reached from the A-site with the three displacement vectors $\mathbf{d}_1 = d(\frac{1}{2}, -\frac{\sqrt{3}}{2})$, $\mathbf{d}_2 = d(\frac{1}{2}, \frac{\sqrt{3}}{2})$, $\mathbf{d}_3 = d(-1,0) = -(\mathbf{d}_1+\mathbf{d}_2)$, where $d = |\mathbf{d}_j|$ is the nearest-neighbor distance. If you call $\mathbf{a}_1 = \mathbf{d}_2 - \mathbf{d}_3 = a(\frac{\sqrt{3}}{2}, \frac{1}{2})$, $\mathbf{a}_2 = \mathbf{d}_3 - \mathbf{d}_1 = a(-\frac{\sqrt{3}}{2}, \frac{1}{2})$ and $\mathbf{a}_3 = \mathbf{d}_1 - \mathbf{d}_2 = -(\mathbf{a}_1+\mathbf{a}_2) = a(0,-1)$, with $a = \sqrt{3}d$, then the next-neighbors of an A-site are again A-sites at the 6 points $\{\pm\mathbf{a}_1, \pm\mathbf{a}_2, \pm\mathbf{a}_3\}$. Similarly for the B sub-lattice. We can take any two of the $\mathbf{a}_i$s, for instance $\mathbf{a}_1$ and $\mathbf{a}_2$, as basis vectors of the Bravais lattice, which will have *two* atoms (an A- and a B-site) in the unit cell. Assuming the hopping matrix elements $h_{\mathbf{r}',\mathbf{r}}$ connect only nearest-neighbor (AB) and next-nearest-neighbor (BB and AA) sites, we can write the Hamiltonian as:

$$\hat{H} = \sum_{\mathbf{r}\in A}\sum_{\mathbf{d}_j}\left(h_{\mathbf{r}+\mathbf{d}_j,\mathbf{r}}\hat{c}^{\dagger}_{\mathbf{r}+\mathbf{d}_j}\hat{c}_{\mathbf{r}} + \text{H.c.}\right) + \sum_{\mathbf{r}}\sum_{\mathbf{a}_j}\left(h_{\mathbf{r}+\mathbf{a}_j,\mathbf{r}}\hat{c}^{\dagger}_{\mathbf{r}+\mathbf{a}_j}\hat{c}_{\mathbf{r}} + \text{H.c.}\right) + \sum_{\mathbf{r}}\epsilon_{\mathbf{r}}\hat{c}^{\dagger}_{\mathbf{r}}\hat{c}_{\mathbf{r}}\,.$$

Haldane [12] considered the possibility that that two sublattices are chemically not equivalent, in which case one might take, without loss of generality, take $\epsilon_{\mathbf{r}\in A} = +M$ and $\epsilon_{\mathbf{r}\in B} = -M$. Haldane also assumed that there is a magnetic field, which will modify the hopping amplitudes according to the Peierls' substitution:

$$h_{\mathbf{r}',\mathbf{r}} \to h^{\mathbf{A}}_{\mathbf{r}',\mathbf{r}} \equiv h_{\mathbf{r}',\mathbf{r}}\, \mathrm{e}^{-i\frac{e}{\hbar c}\int_{\mathbf{r}}^{\mathbf{r}'}\mathbf{A}\cdot d\mathbf{l}}\,, \tag{4.21}$$

More precisely, he assumed that the total flux of the magnetic field over every hexagon of the lattice is *zero*. [8] This means that the line-integral of the vector potential $\mathbf{A}$ around the hexagon has to be zero, and therefore, by $2\pi/3$-rotational symmetry, the line-integral of $\mathbf{A}$ on *every nearest-neighbor bond vanishes*: hence $\mathbf{A}_{\mathbf{r}+\mathbf{d}_j,\mathbf{r}} = 0$ and the nearest-neighbor hopping is not modified at all by the magnetic field. We denote $h^{\mathbf{A}}_{\mathbf{r}+\mathbf{d}_j,\mathbf{r}} = t_1$, where t_1 is a real hopping amplitude. [9] The next-nearest-neighbor hoppings, instead, *are modified* by the magnetic field. If you look at Fig. 4.2, you realize that the line-integral of $\mathbf{A}$ along each (dashed) triangular path in the direction of the arrows (clockwise) has to be *negative*, i.e., $-\Phi_T$, where $\Phi_T > 0$ is the flux through the each triangle; [10] hence, again by rotational symmetry, a phase-factor $\mathrm{e}^{+i(e/\hbar c)\Phi_T/3} = \mathrm{e}^{i2\pi\Phi_T/(3\phi_0)} = \mathrm{e}^{i\phi}$ is associated to each hopping amplitude in the direction of the arrows: here we have introduced the shorthand notation $\phi = 2\pi\Phi_T/(3\phi_0)$, $\phi_0 = hc/e$ being here (twice) the flux quantum, in cgs units. A closer inspection of Fig. 4.2 reveals that this makes the second-neighbor hoppings $h^{\mathbf{A}}_{\mathbf{r}+\mathbf{a}_j,\mathbf{r}} = t_2\mathrm{e}^{\pm i\phi}$ where the $+$ sign applies to the $\mathbf{r}\in A$, and the $-$ sign to the $\mathbf{r}\in B$. We write this, with a slightly baroque notation, [11] as $t_2\mathrm{e}^{i\phi\nu_{\mathbf{r}\to\mathbf{r}+\mathbf{a}_j}}$, where $\nu_{\mathbf{r}\to\mathbf{r}+\mathbf{a}_j} = +1$ if $\mathbf{r}\in A$ and $\nu_{\mathbf{r}\to\mathbf{r}+\mathbf{a}_j} = -1$ if $\mathbf{r}\in B$. We also denote $M_{\mathbf{r}} = \pm M$, where the $+$ applies to $\mathbf{r}\in A$, and the $-$ to $\mathbf{r}\in B$. We

[8] The present footnote is written in SI units because I find them easier to calculate numerical estimates. The argument by Haldane is as follows: if you put a magnetic moment $\boldsymbol{\mu}$ at the center of each hexagon, all of them pointing *up* in the $\hat{\mathbf{z}}$ direction, i.e., ferromagnetically arranged, then the magnetic field (in SI units, with $\frac{\mu_0}{4\pi} = 10^{-7}$ N/A^2) produced by each moment

$$\mathbf{B} = \frac{\mu_0}{4\pi}\frac{1}{r^3}[3(\boldsymbol{\mu}\cdot\hat{\mathbf{r}})\hat{\mathbf{r}} - \boldsymbol{\mu}] \qquad \longrightarrow \qquad -\frac{\mu_0}{4\pi}\frac{|\boldsymbol{\mu}|}{r^3}\hat{\mathbf{z}}\,,$$

will point *down* at any point on the plane. However, the total flux across the plane generated by each single $\boldsymbol{\mu}$ must be 0. (The negative flux away from $\boldsymbol{\mu}$ is compensated by a strong positive δ-like contribution at the location of the magnetic moment, since field lines must be closed.) Therefore, while the flux produced by a single $\boldsymbol{\mu}$ is still positive if you restrict the integral to the hexagon where $\boldsymbol{\mu}$ is located, the negative contribution from all the other moments will necessarily create a field distribution that has *zero* flux when integrated over every hexagon, and with all the symmetries of the lattice. Let us try to estimate this effect. The total negative flux produced by a single $\boldsymbol{\mu}$ on the plane, from a distance r_c to ∞, is $\Phi(r_c,\infty) = -\frac{\mu_0}{4\pi}\frac{2\pi|\boldsymbol{\mu}|}{r_c}$. The positive flux produced by $\boldsymbol{\mu}$ within a region of radius r_c must be just the opposite of this. If $r_c = d = 1.42$ Å $= 2.4a_B$ is the graphene nearest-neighbor distance d, and $|\boldsymbol{\mu}| = \mu_B = \frac{e\hbar}{2m} = 9.274\times10^{-24}$ J/T is the Bohr magneton (in SI units, where J/T=A m^2 is the unit of magnetic moment), you can estimate the flux produced *inside* the hexagon in which $\boldsymbol{\mu}$ is contained as $-\Phi(d,\infty)\approx 0.46\times10^{-19}$ Wb, where Wb=Tm^2 is the SI unit of flux. If you recall that the flux quantum is, in SI, $\phi_0 = \frac{\hbar}{2e} = 2.07\times10^{-15}$ Wb, you realize that these are small effects. Nevertheless, the effect predicted by Haldane has been experimentally observed in 2013 [13], in ferromagnetic Topological Insulators, and is known as Quantum Anomalous Hall Effect (QAHE).

[9] $t_1 \approx -2.8$ eV for graphene.

[10] The flux Φ_T through these triangular paths is positive, hence the line-integral of $\mathbf{A}$ in the *counter-clockwise* direction is positive.

[11] I introduce here this notation to make a bridge with the notation used by Kane and Mele [14] in their discussion of the spin-orbit coupling, and the Spin Quantum Hall effect, in graphene. Kane and Mele call ν_{ij} what we call here $\nu_{\mathbf{r}\to\mathbf{r}+\mathbf{a}_j}$ with the identification $\mathbf{r}\leftrightarrow i$, $\mathbf{r}+\mathbf{a}_j\leftrightarrow j$. With our sign convention, we

therefore write the *Haldane model* as: [12]

$$\hat{H}_{\rm Hal} = \underbrace{t_1 \sum_{\mathbf{r}\in A}\sum_{\mathbf{d}_j}\left(\hat{c}^\dagger_{\mathbf{r}+\mathbf{d}_j}\hat{c}_{\mathbf{r}} + \text{H.c.}\right)}_{\hat{H}_{\rm nn}} + \underbrace{t_2 \sum_{\mathbf{r}}\sum_{\mathbf{a}_j}\left(\mathrm{e}^{i\phi\nu_{\mathbf{r}\to\mathbf{r}+\mathbf{a}_j}}\hat{c}^\dagger_{\mathbf{r}+\mathbf{a}_j}\hat{c}_{\mathbf{r}} + \text{H.c.}\right)}_{\hat{H}_{\rm nnn}} + \underbrace{\sum_{\mathbf{r}} M_{\mathbf{r}}\hat{c}^\dagger_{\mathbf{r}}\hat{c}_{\mathbf{r}}}_{\hat{H}_{\rm site}} \ . \tag{4.23}$$

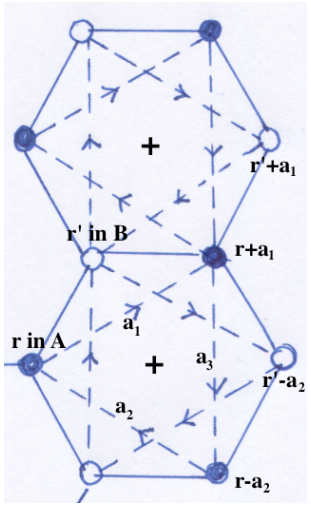

Figure 4.2.: The magnetic fluxes in the Haldane model. See text for details.

We construct the reciprocal lattice vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ in the standard way, i.e., such that $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$. One finds $\mathbf{b}_1 = \frac{4\pi}{\sqrt{3}a}(\frac{1}{2}, \frac{\sqrt{3}}{2})$, and $\mathbf{b}_2 = \frac{4\pi}{\sqrt{3}a}(\frac{1}{2}, -\frac{\sqrt{3}}{2})$, see Fig. 4.1(right), where a possible choice of the Brillouin Zone (BZ) is shown.

When periodic boundary conditions (PBC) are applied in all directions, one can fully exploit translational invariance, defining the Bloch-Wannier transformations:

$$\begin{cases} \hat{c}^\dagger_{\mathbf{k}B} = \dfrac{1}{\sqrt{N}}\displaystyle\sum_{\mathbf{r}\in B}\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\hat{c}^\dagger_{\mathbf{r}} \\ \hat{c}^\dagger_{\mathbf{k}A} = \dfrac{1}{\sqrt{N}}\displaystyle\sum_{\mathbf{r}\in A}\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\hat{c}^\dagger_{\mathbf{r}} \end{cases} \qquad \begin{cases} \hat{c}^\dagger_{\mathbf{r}\in B} = \dfrac{1}{\sqrt{N}}\displaystyle\sum_{\mathbf{k}\in \rm BZ}\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}}\hat{c}^\dagger_{\mathbf{k}B} \\ \hat{c}^\dagger_{\mathbf{r}\in A} = \dfrac{1}{\sqrt{N}}\displaystyle\sum_{\mathbf{k}\in \rm BZ}\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}}\hat{c}^\dagger_{\mathbf{k}A} \end{cases} \tag{4.24}$$

could express this factor

$$\nu_{\mathbf{r}\to\mathbf{r}+\mathbf{a}_j} = -\frac{2}{\sqrt{3}}\left[\mathbf{d}_\alpha \times \mathbf{d}_\beta\right]_z \ ,$$

where $\mathbf{d}_\alpha$ and $\mathbf{d}_\beta$ are, *in that order*, the $\mathbf{d}_{i=1,2,3}$ nearest-neighbor vectors that you have to sum to $\mathbf{r}$ to obtain $\mathbf{r}+\mathbf{a}_j$. It is simple to verify that, if $\mathbf{r} \in A$ then $\nu_{\mathbf{r}\to\mathbf{r}+\mathbf{a}_1} = \frac{2}{\sqrt{3}}\left[\mathbf{d}_2 \times \mathbf{d}_3\right]_z = +1$, $\nu_{\mathbf{r}\to\mathbf{r}+\mathbf{a}_2} = \frac{2}{\sqrt{3}}\left[\mathbf{d}_3 \times \mathbf{d}_1\right]_z = +1$, $\nu_{\mathbf{r}\to\mathbf{r}+\mathbf{a}_3} = \frac{2}{\sqrt{3}}\left[\mathbf{d}_1 \times \mathbf{d}_2\right]_z = +1$, corresponding to the fact that you always take a first step (for instance by $\mathbf{d}_2$), and then you make a *right turn* in the second step (for instance $-\mathbf{d}_3$). For $\mathbf{r} \in B$ you have instead $\nu_{\mathbf{r}\to\mathbf{r}+\mathbf{a}_1} = \frac{2}{\sqrt{3}}\left[\mathbf{d}_3 \times \mathbf{d}_2\right]_z = -1$, and cyclic permutations, corresponding to always making a *left turn* in the second step.

[12] We also report the explicit expression for the corresponding current operator $\hat{\mathbf{J}}$:

$$\hat{\mathbf{J}} = \underbrace{\frac{t_1}{\hbar}\sum_{\mathbf{r}\in A}\sum_{\mathbf{d}_j}\left[(-i\mathbf{d}_j)\hat{c}^\dagger_{\mathbf{r}+\mathbf{d}_j}\hat{c}_{\mathbf{r}} + \text{H.c.}\right]}_{\hat{\mathbf{J}}_{\rm nn}} + \underbrace{\frac{t_2}{\hbar}\sum_{\mathbf{r}}\sum_{\mathbf{a}_j}\left[(-i\mathbf{a}_j)\mathrm{e}^{i\phi\nu_{\mathbf{r}\to\mathbf{r}+\mathbf{a}_j}}\hat{c}^\dagger_{\mathbf{r}+\mathbf{a}_j}\hat{c}_{\mathbf{r}} + \text{H.c.}\right]}_{\hat{\mathbf{J}}_{\rm nnn}} \ . \tag{4.22}$$

Here $N = N_1 N_2$ is the number of unit cells, constructed for instance from $\mathbf{a}_1$ and $\mathbf{a}_2$, making-up a big periodically-repeated lattice (i.e., wrapped-up on a torus in both directions): as a consequence, the *discrete* wave-vectors allowed are

$$\mathbf{k} = \frac{n_1}{N_1}\mathbf{b}_1 + \frac{n_2}{N_2}\mathbf{b}_2 \quad \text{with} \quad n_1, n_2 \in \mathbb{Z}\,, \tag{4.25}$$

with the understanding that only N of them are independent; for instance $n_1 = 0 \cdots N_1 - 1$ and $n_2 = 0 \cdots N_2 - 1$ make up a possible choice of independent $\mathbf{k}$-points, as shown in the rhombic BZ of Fig. 4.1(right). Inserting these expressions in the Haldane model, we can transform it in the form:

$$\hat{H}_{\rm Hal} = \sum_{\mathbf{k}}^{\rm BZ} \left[\hat{c}^\dagger_{\mathbf{k}A}\ \hat{c}^\dagger_{\mathbf{k}B}\right] \left[\hat{\mathcal{H}}(\mathbf{k})\right] \begin{bmatrix} \hat{c}_{\mathbf{k}A} \\ \hat{c}_{\mathbf{k}B} \end{bmatrix} \tag{4.26}$$

where, for each $\mathbf{k} \in$ BZ, the Hamiltonian $\hat{\mathcal{H}}(\mathbf{k})$ is a 2×2 Hermitean matrix, which one can always parameterize, in terms of the identity $\mathbb{1}$ and the three Pauli matrices $\hat{\boldsymbol{\sigma}}$, as $\hat{\mathcal{H}}(\mathbf{k}) = R_0(\mathbf{k})\,\mathbb{1} + \mathbf{R}(\mathbf{k}) \cdot \hat{\boldsymbol{\sigma}}$, or, more explicitly, as:

$$\hat{\mathcal{H}}(\mathbf{k}) = \begin{bmatrix} H_{11}(\mathbf{k}) & H_{12}(\mathbf{k}) \\ H^*_{12}(\mathbf{k}) & H_{22}(\mathbf{k}) \end{bmatrix} = R_0(\mathbf{k})\,\mathbb{1} + R_x(\mathbf{k})\hat{\sigma}_x + R_y(\mathbf{k})\hat{\sigma}_y + R_z(\mathbf{k})\hat{\sigma}_z \tag{4.27}$$

with $H_{11} = R_0 + R_z$, $H_{22} = R_0 - R_z$, and $H_{12} = R_x - iR_y$. It turns out that, if you actually perform the calculation [13] with the specific choice of $\hat{c}^\dagger_{\mathbf{k}B}$ written above, you would find that

$$R_0(\mathbf{k}) = 2t_2(\cos\phi)\sum_{j=1}^{3}\cos\left(\mathbf{k}\cdot\mathbf{a}_j\right) \quad \text{and} \quad R_z(\mathbf{k}) = M + 2t_2(\sin\phi)\sum_{j=1}^{3}\sin\left(\mathbf{k}\cdot\mathbf{a}_j\right)\,, \tag{4.28}$$

which is nice, because the direct lattice vectors $\mathbf{a}_j$ appear: hence $R_{0/z}(\mathbf{k}+\mathbf{G}) = R_{0/z}(\mathbf{k})$ for any reciprocal lattice vector $\mathbf{G} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2$. However, with this choice of $\hat{c}^\dagger_{\mathbf{k}B}$ you would

[13] Here is sketch of what you do. For the t_1-term:

$$\hat{H}_{\rm nn} = \frac{t_1}{N}\sum_{\mathbf{r}\in A}\sum_{j=1}^{3}\sum_{\mathbf{k},\mathbf{k}'}^{\rm BZ}\left[\mathrm{e}^{-i\mathbf{k}'\cdot(\mathbf{r}+\mathbf{d}_j)}\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\hat{c}^\dagger_{\mathbf{k}'B}\hat{c}_{\mathbf{k}A} + \text{H.c.}\right] = t_1\sum_{\mathbf{k}}^{\rm BZ}\left[\left(\sum_{j=1}^{3}\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{d}_j}\right)\hat{c}^\dagger_{\mathbf{k}B}\hat{c}_{\mathbf{k}A} + \text{H.c.}\right]\,,$$

where we exploit the Krönecker delta:

$$\frac{1}{N}\sum_{\mathbf{r}\in A}\mathrm{e}^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} = \delta_{\mathbf{k},\mathbf{k}'}\,.$$

For the t_2-term, separating the A and B sublattice contributions, we have:

$$\begin{aligned}\hat{H}_{{\rm nnn}A/B} &= \frac{t_2}{N}\sum_{\mathbf{r}\in A/B}\sum_{j=1}^{3}\sum_{\mathbf{k},\mathbf{k}'}^{\rm BZ}\left[\mathrm{e}^{\pm i\phi}\mathrm{e}^{-i\mathbf{k}'\cdot(\mathbf{r}+\mathbf{a}_j)}\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\hat{c}^\dagger_{\mathbf{k}'A/B}\hat{c}_{\mathbf{k}A/B} + \text{H.c.}\right] \\ &= t_2\sum_{\mathbf{k}}^{\rm BZ}\left[\left(\sum_{j=1}^{3}\mathrm{e}^{\pm i\phi}\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{a}_j}\right)\hat{c}^\dagger_{\mathbf{k}A/B}\hat{c}_{\mathbf{k}A/B} + \text{H.c.}\right]\end{aligned}$$

For the (on-site) M-term, again separating A and B:

$$\hat{H}_{{\rm site}A/B} = \pm M\frac{1}{N}\sum_{\mathbf{r}\in A/B}\sum_{\mathbf{k},\mathbf{k}'}^{\rm BZ}\left[\mathrm{e}^{-i\mathbf{k}'\cdot\mathbf{r}}\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\hat{c}^\dagger_{\mathbf{k}'A/B}\hat{c}_{\mathbf{k}A/B}\right] = \pm M\sum_{\mathbf{k}}^{\rm BZ}\left[\hat{c}^\dagger_{\mathbf{k}A/B}\hat{c}_{\mathbf{k}A/B}\right]\,.$$

get $R_x(\mathbf{k}) - iR_y(\mathbf{k}) = t_1 \sum_{j=1}^{3} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{d}_j}$, i.e.:

$$R_x(\mathbf{k}) = t_1 \sum_{j=1}^{3} \cos(\mathbf{k}\cdot\mathbf{d}_j) \quad \text{and} \quad R_y(\mathbf{k}) = t_1 \sum_{j=1}^{3} \sin(\mathbf{k}\cdot\mathbf{d}_j) \tag{4.29}$$

which is not infinitely satisfactory, because $R_{x/y}(\mathbf{k}+\mathbf{G}) \neq R_{x/y}(\mathbf{k})$. This makes absolutely no difference if you are simply interested in the *band dispersion* (it contributes irrelevant phase factors), but it proves inconvenient in the present context of calculating the Chern number, because we would like to have $\widetilde{\mathbf{R}}(\mathbf{k}+\mathbf{G}) = \widetilde{\mathbf{R}}(\mathbf{k})$ in such a way that the mapping from the BZ to the $\mathbf{R}$-space is actually *periodic* over the BZ. If you really insist in having a periodic $\widetilde{\mathbf{R}}(\mathbf{k}+\mathbf{G}) = \widetilde{\mathbf{R}}(\mathbf{k})$ then there is a simple way out, however. Simply make, for instance, a canonical transformation

$$\hat{c}^\dagger_{\mathbf{k}B} \to \tilde{c}^\dagger_{\mathbf{k}B} = \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{d}_3}\hat{c}^\dagger_{\mathbf{k}B} = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}\in B} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{d}_3)}\hat{c}^\dagger_{\mathbf{r}} \,, \tag{4.30}$$

with the inverse transformation now reading:

$$\hat{c}^\dagger_{\mathbf{r}\in B} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\in \mathrm{BZ}} \mathrm{e}^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{d}_3)}\tilde{c}^\dagger_{\mathbf{k}B} \,, \tag{4.31}$$

and this will make: [14]

$$\widetilde{R}_x(\mathbf{k}) = t_1 \left[1 + \cos(\mathbf{k}\cdot\mathbf{a}_1) + \cos(\mathbf{k}\cdot\mathbf{a}_2)\right] \quad \text{and} \quad \widetilde{R}_y(\mathbf{k}) = t_1 \left[\sin(\mathbf{k}\cdot\mathbf{a}_2) - \sin(\mathbf{k}\cdot\mathbf{a}_1)\right] \,, \tag{4.32}$$

which has the desired periodicity $\mathbf{k} \to \mathbf{k} + \mathbf{G}$. [15]

Diagonalizing $\hat{\mathcal{H}}(\mathbf{k})$ for any given $\mathbf{k} \in$ BZ is a simple spin-1/2 problem. The two eigenvalues are

$$\epsilon_{\mathbf{k}\pm} = R_0(\mathbf{k}) \pm |\mathbf{R}(\mathbf{k})| \,. \tag{4.34}$$

The two eigenvectors are exactly the two spinors we have discussed for the spin-1/2 problem, for which the story of the choice of the phase and the unavoidable presence of vortex singularities applies as well (see discussion in Sec. 3.4). Let us denote by $|u_{\mathbf{k}\pm}\rangle$ the spinors corresponding to the two bands. Notice that we can parameterize them by simply knowing the angles $\theta_{\mathbf{k}}$ and $\phi_{\mathbf{k}}$ that the "magnetic field" $\mathbf{R}(\mathbf{k})$ has on the (Bloch) sphere in spin space. In all cases, unless the parameters are specially tuned (see below) the two bands are separated by a gap, which implies that the system is an insulator if the number of particles is so chosen that the lower band is completely filled and the upper band is empty: for that, you need a half-filling situation, i.e., the number of electrons has to be half the number of

[14] Simply notice that now:

$$\hat{H}_{\mathrm{nn}} = \frac{t_1}{N} \sum_{\mathbf{r}\in A} \sum_{j=1}^{3} \sum_{\mathbf{k},\mathbf{k}'}^{\mathrm{BZ}} \left[\mathrm{e}^{-i\mathbf{k}'\cdot(\mathbf{r}+\mathbf{d}_j-\mathbf{d}_3)}\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\tilde{c}^\dagger_{\mathbf{k}'B}\hat{c}_{\mathbf{k}A} + \mathrm{H.c.}\right] = t_1 \sum_{\mathbf{k}}^{\mathrm{BZ}} \left[\left(\sum_{j=1}^{3} \mathrm{e}^{-i\mathbf{k}\cdot(\mathbf{d}_j-\mathbf{d}_3)}\right)\tilde{c}^\dagger_{\mathbf{k}B}\hat{c}_{\mathbf{k}A} + \mathrm{H.c.}\right] \,,$$

and recall that $\mathbf{d}_2 - \mathbf{d}_3 = \mathbf{a}_1$ and $\mathbf{d}_1 - \mathbf{d}_3 = -\mathbf{a}_2$. Equivalently, observe that $(R_x - iR_y)\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{d}_3} = \widetilde{R}_x - i\widetilde{R}_y$.

[15] Expanding $\widetilde{R}_x(\mathbf{k}) - i\widetilde{R}_y(\mathbf{k})$ near the two Dirac points, taking $\mathbf{k} = \mathbf{K}_\pm + \mathbf{q}$, you get:

$$\widetilde{R}_x(\mathbf{K}_\pm + \mathbf{q}) - i\widetilde{R}_y(\mathbf{K}_\pm + \mathbf{q}) = i\frac{\sqrt{3}t_1 a}{2}\Big[q_x \mp iq_y\Big] \,. \tag{4.33}$$

available orbitals (lattice sites, if you neglect spin, as we are doing). The crucial point (we will see this, with illustrations, later on, don't worry) will be *if*, when $\mathbf{k}$ spans over the BZ of the lattice (a torus, due to PBC), this "magnetic field" $\mathbf{R}(\mathbf{k})$ will *wrap around the origin* of the Bloch sphere in spin-space or not. In the second case, we will see that the insulator is a trivial insulator; in the first case, it is not. More about this, in connection with the physics of the Hall conductivity in the Haldane model, in section 4.4. [16]

Returning to the discussion of the band dispersion, we find band degeneracies at the $\mathbf{k}$ points where $\mathbf{R}(\mathbf{k}) = \mathbf{0}$: if you go back to the discussion about the spin-1/2 in a magnetic field in Sec. 3.4, you realize that degeneracies occur exactly where the magnetic field vanishes, $\mathbf{R}^* = \mathbf{0}$. When $M = 0$ and $\phi = 0$, the standard graphene case (where one usually puts $t_2 = 0$ as well), these degeneracies occur at the two famous *Dirac points*, located at the hexagonal-BZ corners, i.e., the two points labeled $\mathbf{K}_1$ and $\mathbf{K}_{-1}$ (or simply $\mathbf{K}_+$ and $\mathbf{K}_-$) in the rhombic-BZ of Fig. 4.1. Defining the label $\alpha = \pm 1$, one finds that $\mathbf{K}_\alpha = \mathbf{K}_\pm = (\frac{2\pi}{\sqrt{3}a}, \pm\frac{2\pi}{3a})$, and is indeed a simple matter to show that $\mathbf{K}_\alpha \cdot \mathbf{a}_j = -\alpha(2\pi/3)$. At the two Dirac points (and only at those points!) one has $R_x(\mathbf{K}_\alpha) = 0$ and $R_y(\mathbf{K}_\alpha) = 0$. [17] Since the presence of a degeneracy requires/implies $\mathbf{R}(\mathbf{k}) = \mathbf{0} \longrightarrow R_{x/y}(\mathbf{k}) = 0$, we immediately conclude that a degeneracy can only occur in one of the two BZ corners $\mathbf{K}_\alpha$. The matter is then decided by what is the value of $R_z(\mathbf{K}_\alpha)$. However, since:

$$\sum_{j=1}^{3} \sin\left(\mathbf{K}_\alpha \cdot \mathbf{a}_j\right) = -\alpha \frac{3\sqrt{3}}{2} \,, \tag{4.36}$$

we see that the presence of degeneracies is all linked to:

$$R_z(\mathbf{K}_\alpha) = M - 3\sqrt{3}\alpha t_2 \sin\phi \equiv 0 \,. \tag{4.37}$$

These two equations, for $\alpha = \pm$, define two curves in the M/t_2 versus ϕ plane, the phase diagram of the Haldane model, where the gap closes *either* at the $\mathbf{K}_+$-point, when $M/t_2 = +3\sqrt{3}\sin(\phi)$, *or* at the $\mathbf{K}_-$-point, when $M/t_2 = -3\sqrt{3}\sin(\phi)$: see Fig. 4.3. Everywhere else in the $M/t_2 - \phi$ plane a gap is present, and the system is therefore an *insulator*.

What type of insulator is exactly the matter now: we will see that *outside* the colored area in Fig. 4.3 we have indeed a trivial band-insulator of the Boron-Nitride (BN) type. *Inside* the colored area in Fig. 4.3, however, $\cdots$ Just keep reading the next two sections.

[16] Since it sometimes useful in the context of calculating the Hall conductivity of our problem, let me mention here that the current operator is readily obtained by noticing that a gradient of $\hat{\mathcal{H}}(\mathbf{k})$ with respect to $\mathbf{k}$ brings down precisely the right factors $(-i\mathbf{d}_j)$ or $(-i\mathbf{a}_j)$ in the current expression. Therefore, with the original choice of phases for the $\hat{c}_{\mathbf{k}B}$s we can compactly write:

$$\hat{\mathbf{J}} = \sum_{\mathbf{k}}^{\mathrm{BZ}} \left(\hat{c}^\dagger_{\mathbf{k}A}\ \hat{c}^\dagger_{\mathbf{k}B}\right) \left(\frac{1}{\hbar}\boldsymbol{\nabla}_{\mathbf{k}}\mathcal{H}(\mathbf{k})\right) \begin{pmatrix} \hat{c}_{\mathbf{k}A} \\ \hat{c}_{\mathbf{k}B} \end{pmatrix} \tag{4.35}$$

Notice that, while the canonical transformation $\hat{c}^\dagger_{\mathbf{k}B} \to \tilde{c}^\dagger_{\mathbf{k}B} = \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{d}_3}\hat{c}^\dagger_{\mathbf{k}B}$ transforms $\hat{\mathcal{H}}(\mathbf{k}) \to \widetilde{\mathcal{H}}(\mathbf{k})$ where $\widetilde{\mathcal{H}}(\mathbf{k}+\mathbf{G}) = \widetilde{\mathcal{H}}(\mathbf{k})$, the previous nice form of the current operator is a bit ruined. I am pretty confident that the physics should be the same in the two pictures, but a discussion of the conductivity is better carried on in the original picture.

[17] It is elementary to check that also $\widetilde{R}_{x/y}(\mathbf{K}_\alpha) = 0$. Indeed, one can show that $|\mathbf{R}(\mathbf{k})| = |\widetilde{\mathbf{R}}(\mathbf{k})|$, i.e., the band dispersion is not modified at all by the canonical transformation, as it should.

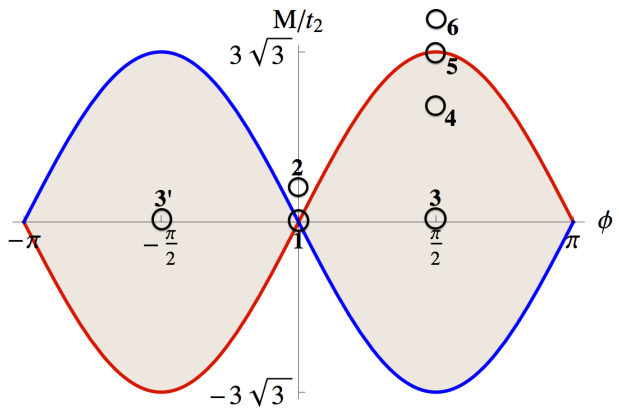

Figure 4.3.: The phase diagram of the Haldane model. Points marked are those for which details are shown in other figures.

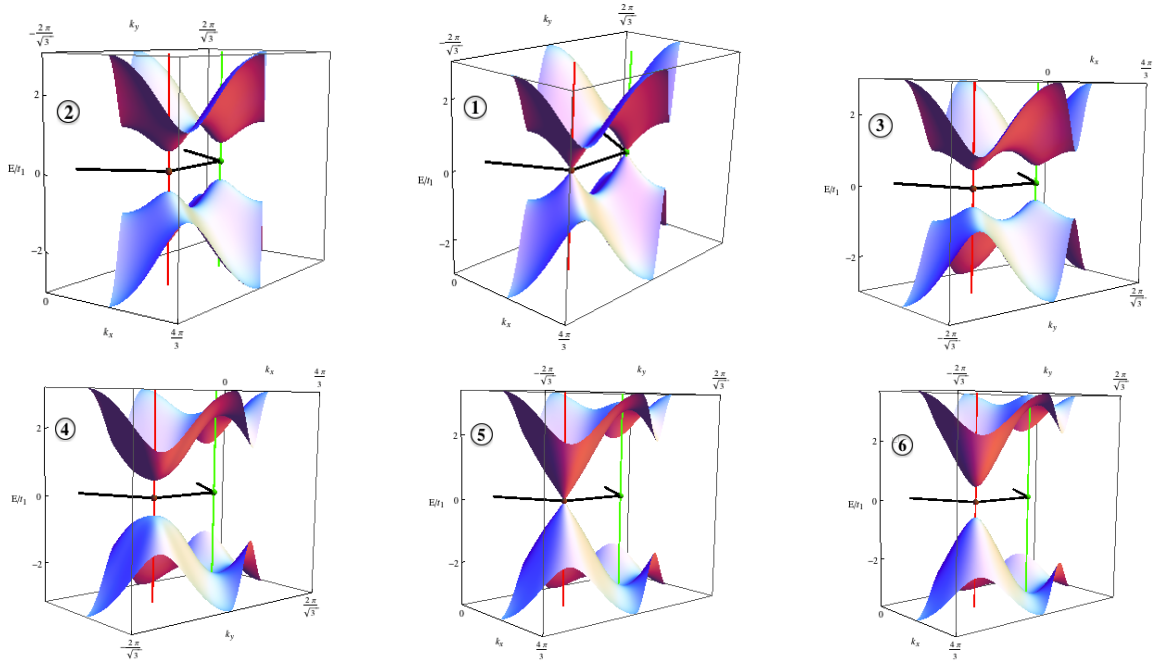

Figure 4.4.: The bands for the Haldane model. Labels refer to the points marked in the phase diagram of Fig. 4.3. The central upper plot shows the two-Dirac bands of standard graphene. The left upper plot is obtained with $M/t_1 = 0.3 \cdot \sqrt{3}$ and $t_2 = 0$ (ordinary BN-type insulator), the right upper plot for $\phi = \pi/2$ with $M = 0$ and $t_2/t_1 = 0.1$ in the topological insulator region. Notice the superficial similarity of the bands in the latter two cases. Lower plots show similar results for points marked 4, 5, and 6 in the phase diagram: notice again the superficial similarity of point 4 and 6.

4.3. The Hall conductivity: A derivation *à la Thouless*

I give here an "adiabatic derivation" of the Hall conductivity — in spirit due to Thouless and followers, see for instance [15, Sec. 4.3] — which clearly shows the role that the Berry curvature plays in transport. This role has been made explicit in the theory of semi-classical transport in crystals by Q. Niu and coworkers. I prefer this derivation to the more traditional one, using linear response theory and Kubo formula, which you can find in Appendix A.

Suppose you have an insulator — which has some magnetic field $\mathbf{B}(\mathbf{x})$ [18] represented by a vector potential $\mathbf{A}$ — and you put an extra uniform-in-space, constant-in-time and *small* electric field $\mathbf{E}$. If you want to keep the Hamiltonian with the same translational invariance it had in absence of $\mathbf{E}$, you better avoid using the scalar potential gauge $\mathbf{E} = -\boldsymbol{\nabla}\phi$, because the resulting scalar potential would break translational invariance. A far more convenient choice is to represent $\mathbf{E}$ in terms of an extra uniform vector potential $\mathbf{A}_E(t)$ such that

$$\mathbf{E} = -\frac{1}{c}\frac{\partial}{\partial t}\mathbf{A}_E(t) \quad \Rightarrow \quad \mathbf{A}_E(t) = -\mathbf{E}\, ct \ . \tag{4.38}$$

This in turn means that, if you are working on the continuum, you should substitute

$$\hat{\mathbf{p}} + \frac{e}{c}\mathbf{A} \to \hat{\mathbf{p}} + \frac{e}{c}\Big[\mathbf{A} + \mathbf{A}_E(t)\Big] = \hat{\mathbf{p}} + \frac{e}{c}\mathbf{A} + \mathbf{R}(t) \ ,$$

where $\mathbf{R}(t) \equiv \hbar\boldsymbol{\kappa}(t) = -e\mathbf{E}\, t$. If you are working with a tight-binding description, then — remember Peierls substitution —

$$h^{\mathbf{A}}_{\mathbf{r}',\mathbf{r}} \to h^{\mathbf{A}}_{\mathbf{r}',\mathbf{r}}\ \mathrm{e}^{-\frac{i}{\hbar}(\mathbf{r}'-\mathbf{r})\cdot\mathbf{R}(t)} \ .$$

In both cases, you realize that $\mathbf{R} = \hbar\boldsymbol{\kappa}$ is a momentum and $\dot{\mathbf{R}} = \hbar\dot{\boldsymbol{\kappa}}$ is the electrical *force* felt by each electron: so, you are essentially *boosting* the momentum of each particle by $\mathbf{R}(t)$, or $\mathbf{k} \to \mathbf{k} + \boldsymbol{\kappa}(t)$. Let us see better, for instance in the continuum case. If you have the Bloch solutions $\psi_{\mathbf{k}}(\mathbf{x}) = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}}u_{\mathbf{k}}(\mathbf{x})$ of the original problem [19]

$$\Big[\frac{1}{2m}\Big(\hat{\mathbf{p}} + \frac{e}{c}\mathbf{A}\Big)^2 + v(\mathbf{x})\Big]\psi_{\mathbf{k}}(\mathbf{x}) = \epsilon_{\mathbf{k}}\psi_{\mathbf{k}}(\mathbf{x}) \ ,$$

then it takes little algebra [20] to show that $\psi_{\mathbf{k}}(\mathbf{x},t) = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}}u_{\mathbf{k}+\boldsymbol{\kappa}(t)}(\mathbf{x})$ solves the instantaneous problem in presence of $\mathbf{R}(t)$, with energy $\epsilon_{\mathbf{k}+\boldsymbol{\kappa}(t)}$:

$$\Big[\frac{1}{2m}\Big(\hat{\mathbf{p}} + \frac{e}{c}\mathbf{A} + \mathbf{R}(t)\Big)^2 + v(\mathbf{x})\Big]\psi_{\mathbf{k}}(\mathbf{x},t) = \epsilon_{\mathbf{k}+\boldsymbol{\kappa}(t)}\ \psi_{\mathbf{k}}(\mathbf{x},t) \ .$$

[18] Generally speaking, the presence of a magnetic field makes the use of Bloch theorem very complex, because the vector potential $\mathbf{A}$ would not respect the discrete translations of the solid; but if you have, as in the Haldane model, a vector potential $\mathbf{A}(\mathbf{x})$ with the full symmetry of the crystal, because the magnetic field has zero flux over every unit cell, then no problem arises.

[19] Then $u_{\mathbf{k}}(\mathbf{x})$ verifies the associated problem

$$\Big[\frac{1}{2m}\Big(\hat{\mathbf{p}} + \frac{e}{c}\mathbf{A} + \hbar\mathbf{k}\Big)^2 + v(\mathbf{x})\Big]u_{\mathbf{k}}(\mathbf{x}) = \epsilon_{\mathbf{k}}u_{\mathbf{k}}(\mathbf{x}) \ ,$$

[20] Simply observe that if you make the *Ansatz* $\psi_{\mathbf{k}}(\mathbf{x},t) = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}}u_{\mathbf{k}+\boldsymbol{\kappa}(t)}(\mathbf{x})$ and substitute it in the Schrödinger equation, then the equation for $u_{\mathbf{k}+\boldsymbol{\kappa}(t)}$ comes out to be

$$\Big[\frac{1}{2m}\Big(\hat{\mathbf{p}} + \frac{e}{c}\mathbf{A} + \hbar(\mathbf{k} + \boldsymbol{\kappa}(t))\Big)^2 + v(\mathbf{x})\Big]u_{\mathbf{k}+\boldsymbol{\kappa}(t)}(\mathbf{x}) = \epsilon_{\mathbf{k}+\boldsymbol{\kappa}(t)}u_{\mathbf{k}+\boldsymbol{\kappa}(t)}(\mathbf{x}) \ ,$$

which is indeed the correct equation that the periodic part has to satisfy, for any fixed instantaneous value of $\boldsymbol{\kappa}(t)$.

In all cases, the price to pay for having translational invariance respected is that the Hamiltonian becomes *time-dependent* $\hat{H} \to \hat{H}(\mathbf{R}(t))$. The notation chosen for $\mathbf{R}(t)$ should remind you of our general discussion of adiabatic theorem: and indeed, if $|\mathbf{E}|$ is small then $\mathbf{R}(t)$ varies *slowly* — equivalently, $\dot{\mathbf{R}} = -e\mathbf{E}$ is small — and if the system we are considering is an *insulator* — hence the initial ground state $|\Phi_0\rangle$ is separated by a finite gap from all other states $|\Phi_n\rangle$ — an adiabatic approach should work. A noteworthy expression which we will eventually use is that, at the operator level, we can always express the total particle current operator as

$$\widehat{\mathbf{J}} = \boldsymbol{\nabla}_{\mathbf{R}} \hat{H}(\mathbf{R}) \; . \tag{4.39}$$

See, for instance, Eq. (4.17) for the tight-binding case.

Our starting point will then be expansion of $|\Psi(t)\rangle$ in terms of instantaneous eigenstates $|\Phi_n(\mathbf{R}(t))\rangle$ of $\hat{H}(\mathbf{R}(t))$ we have written when discussing the adiabatic theorem: [21]

$$|\Psi(t)\rangle = \sum_n c_n(t)\, \mathrm{e}^{i\gamma_n(t)}\, \mathrm{e}^{-\frac{i}{\hbar}\int_0^t dt' E_n(t')}\, |\Phi_n(t)\rangle \; , \tag{4.40}$$

where the initial condition is $c_n(0) = \delta_{n,0}$, with the compact notation $E_n(t) \equiv E_n(\mathbf{R}(t))$, and $\Phi_n(t) \equiv \Phi_n(\mathbf{R}(t))$. You will remember, see Eq. (3.10), that we derived the following system of differential equations for the $c_n(t)$:

$$\dot{c}_n(t) = \sum_{m \neq n} \mathrm{e}^{\frac{i}{\hbar}\int_0^t dt' [E_n(t') - E_m(t')]}\, F_{nm}(t)\, c_m(t) \; , \tag{4.41}$$

where the coefficients $F_{nm}(t)$ are given by $F_{nm}(t) = -\mathrm{e}^{i[\gamma_m(t)-\gamma_n(t)]}\, \dot{\mathbf{R}} \cdot \langle \Phi_n | \boldsymbol{\nabla}_{\mathbf{R}} \Phi_m \rangle$, or equivalently:

$$F_{nm}(t) = -\mathrm{e}^{i[\gamma_m(t)-\gamma_n(t)]}\, \langle \Phi_n(t) | \partial_t \Phi_m(t) \rangle \; . \tag{4.42}$$

Eq. (4.41) is the starting point for an obvious *perturbative expansion*, where you substitute the $c_m(t)$ appearing on the right-hand-side with some order-k approximation $c_m^{(k)}(t)$ to get the $c_n^{(k+1)}(t)$ on the left-hand-side to order $k+1$. To lowest order, $c_m^{(0)}(t) = c_m(0) = \delta_{m,0}$, hence we can write the following *first-order* expression:

$$\dot{c}_n^{(1)}(t) = (1 - \delta_{n,0})\, \mathrm{e}^{\frac{i}{\hbar}\int_0^t dt' [E_n(t') - E_0(t')]}\, F_{n0}(t) \; , \tag{4.43}$$

Integrating over time, by parts, we can then write:

$$c_n^{(1)}(t) = -i\hbar(1-\delta_{n,0}) \left[\frac{\mathrm{e}^{\frac{i}{\hbar}\int_0^t dt' [E_n(t') - E_0(t')]}}{E_n(t) - E_0(t)}\, F_{n0}(t) + \cdots - \int_0^t dt' \, \frac{\mathrm{e}^{\frac{i}{\hbar}\int_0^{t'} dt'' [E_n(t'') - E_0(t'')]}}{E_n(t') - E_0(t')}\, \dot{F}_{n0}(t') \right] ,$$

where the $\cdots$ collect a term which comes from the derivative of the denominator $E_n(t) - E_0(t)$, which we are neglecting. The final term in the previous expression contains a time derivative of F_{n0} and is therefore less relevant in the adiabatic regime we have in mind. Keeping only the first term, we finally write an approximate expression for the state $|\Psi(t)\rangle$, to first-order in the time-derivatives, as follows:

$$|\Psi(t)\rangle = \mathrm{e}^{i\gamma_0(t)}\, \mathrm{e}^{-\frac{i}{\hbar}\int_0^t dt' E_0(t')} \left[|\Phi_0(t)\rangle + i\hbar \sum_{n \neq 0} \frac{|\Phi_n(t)\rangle \langle \Phi_n(t) | \partial_t \Phi_0(t) \rangle}{E_n(t) - E_0(t)} \right] , \tag{4.44}$$

[21] Notice that we switch back to t here, rather then using $s = t/T$.

which coincides with Eq. (2.3) of Ref. [8]. The second term contains an important correction to the adiabatic state which will play a crucial role in transport, as we shall presently see.

Consider the total particle current $\widehat{\mathbf{J}} = \boldsymbol{\nabla}_{\mathbf{R}}\hat{H}$ and evaluate its average over $|\Psi(t)\rangle$. You will get, to lowest order in the corrections to adiabaticity, two contributions:

$$\langle\Psi(t)|\widehat{\mathbf{J}}|\Psi(t)\rangle = \langle\Phi_0(t)|\boldsymbol{\nabla}_{\mathbf{R}}\hat{H}|\Phi_0(t)\rangle + i\hbar\sum_{n\neq 0}\left[\frac{\langle\Phi_0(t)|\boldsymbol{\nabla}_{\mathbf{R}}\hat{H}|\Phi_n(t)\rangle\langle\Phi_n(t)|\partial_t\Phi_0(t)\rangle}{E_n(t)-E_0(t)} - \text{c.c.}\right] .$$

You recognize in the first term, through the Hellmann-Feynman relationship, the derivative of the total "ground state" energy $E_0(\mathbf{R}(t))$:

$$\langle\Phi_0(t)|\boldsymbol{\nabla}_{\mathbf{R}}\hat{H}(\mathbf{R}(t))|\Phi_0(t)\rangle = \boldsymbol{\nabla}_{\mathbf{R}}\langle\Phi_0(t)|\hat{H}(\mathbf{R}(t))|\Phi_0(t)\rangle = \boldsymbol{\nabla}_{\mathbf{R}}E_0(\mathbf{R}(t)) .$$

In the second term we recognize a familiar face, see Eq. (3.13)

$$\frac{\langle\Phi_0(t)|\boldsymbol{\nabla}_{\mathbf{R}}\hat{H}|\Phi_n(t)\rangle}{E_n(t)-E_0(t)} = -\langle\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(t)|\Phi_n(t)\rangle ,$$

valid for all $n \neq 0$. Whence we get:

$$\begin{aligned}\langle\Psi(t)|\widehat{\mathbf{J}}|\Psi(t)\rangle &= \boldsymbol{\nabla}_{\mathbf{R}}E_0 - i\hbar\sum_{n\neq 0}\left[\langle\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(t)|\Phi_n(t)\rangle\langle\Phi_n(t)|\partial_t\Phi_0(t)\rangle - \text{c.c.}\right] \qquad (4.45)\\ &= \boldsymbol{\nabla}_{\mathbf{R}}E_0 - i\hbar\Big[\langle\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(t)|\partial_t\Phi_0(t)\rangle - \text{c.c.}\Big] ,\end{aligned}$$

where in the final step we have used the fact that a term with $n = 0$ can be freely added because it is *real* hence it cancels when you subtract the complex conjugate; hence the whole unrestricted sum over n can be eliminated, since it is an identity. Now, recall that $\mathbf{R}(t)$ simply boosts every momentum by $\mathbf{R}(t)$. But in an band insulator all momenta are either completely filled, or empty: hence $E_0(\mathbf{R}(t))$ *does not depend* on $\mathbf{R}(t)$ at all. For a band insulator, therefore, the only remaining term of the electric current is:

$$\langle\Psi(t)|\widehat{\mathrm{J}}_\alpha|\Psi(t)\rangle = -i\hbar\Big[\langle\partial_\alpha\Phi_0|\partial_t\Phi_0\rangle - \langle\partial_t\Phi_0|\partial_\alpha\Phi_0\rangle\Big] . \qquad (4.46)$$

But $|\partial_t\Phi_0\rangle = \dot{\mathbf{R}}\cdot|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0\rangle$ and $\dot{\mathbf{R}} = -e\mathbf{E}$. Inserting into the previous expression we finally get:

$$\langle\Psi(t)|\widehat{\mathrm{J}}_\alpha|\Psi(t)\rangle = ie\hbar\sum_\beta\Big[\langle\partial_\alpha\Phi_0|\partial_\beta\Phi_0\rangle - \langle\partial_\beta\Phi_0|\partial_\alpha\Phi_0\rangle\Big]\,E_\beta . \qquad (4.47)$$

Now recall that the average electric current density is given by

$$\mathrm{j}^e_\alpha = \frac{-e}{\mathrm{Vol}}\langle\Psi(t)|\widehat{\mathrm{J}}_\alpha|\Psi(t)\rangle ,$$

and the conductivity $\sigma_{\alpha\beta}$ is defined from the relationship $\mathrm{j}^e_\alpha = \sum_\beta\sigma_{\alpha\beta}E_\beta$. Inserting all the factors we finally get that the conductivity tensor of a band insulator must be:

$$\sigma_{\alpha\beta} = -\frac{e^2\hbar}{\mathrm{Vol}}i\Big[\langle\partial_\alpha\Phi_0|\partial_\beta\Phi_0\rangle - \langle\partial_\beta\Phi_0|\partial_\alpha\Phi_0\rangle\Big] . \qquad (4.48)$$

This expression clearly shows the crucial role played by the *Berry curvature*. Notice that $\sigma_{\alpha\alpha} = 0$ — the longitudinal conductivity must vanish — and $\sigma_{\alpha\beta} = -\sigma_{\beta\alpha}$ — the transverse conductivity is antisymmetric.

Let us make this expression more explicit by using translational invariance and the fact that we deal with an independent particle Hamiltonian. If $\mathbf{k}$ are the wave-vectors of the Bloch states, and n the (filled) band index, then the initial state is a Slater determinant, which in second quantization reads:

$$|\Phi_0(0)\rangle = \prod_{\mathbf{k}}^{\text{BZ}} \prod_{n}^{\text{filled}} \hat{c}^\dagger_{n\mathbf{k}}|0\rangle \ , \tag{4.49}$$

where $\hat{c}^\dagger_{n\mathbf{k}}$ are the creation operators of Bloch states, and $\psi_{n\mathbf{k}}(\mathbf{x}) = \langle \mathbf{x}|\hat{c}^\dagger_{n\mathbf{k}}|0\rangle$. Correspondingly, the instantaneous ground state in presence of $\mathbf{R}(t)$ is the Slater determinant:

$$|\Phi_0(t)\rangle = \prod_{\mathbf{k}}^{\text{BZ}} \prod_{n}^{\text{filled}} \hat{c}^\dagger_{n\mathbf{k}}(t)|0\rangle \ ,$$

where $\langle \mathbf{x}|\hat{c}^\dagger_{n\mathbf{k}}(t)|0\rangle = \psi_{n\mathbf{k}}(\mathbf{x},t) = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}} u_{n\mathbf{k}+\boldsymbol{\kappa}(t)}(\mathbf{x})$, with instantaneous energy

$$E_0(t) = \sum_{\mathbf{k}}^{\text{BZ}} \sum_{n}^{\text{filled}} \epsilon_{n\mathbf{k}+\boldsymbol{\kappa}(t)} \ .$$

Clearly, in the thermodynamic limit E_0 does not depend at all on $\mathbf{R}$, as previously discussed. Now we should take derivatives with respect to $\mathbf{R}$ to calculate the Berry curvature. Suppose we had a single particle. Then, in first quantization language we should calculate $[\langle \partial_{R_\alpha}\psi_{n\mathbf{k}}|\partial_{R_\beta}\psi_{n\mathbf{k}}\rangle - \langle \partial_{R_\beta}\psi_{n\mathbf{k}}|\partial_{R_\alpha}\psi_{n\mathbf{k}}\rangle]$. But:

$$\partial_{R_\alpha}\psi_{n\mathbf{k}} = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}}\ \partial_{R_\alpha} u_{n\mathbf{k}+\mathbf{R}/\hbar} = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}}\ \frac{1}{\hbar}\partial_{k_\alpha} u_{n\mathbf{k}+\mathbf{R}/\hbar} \ ,$$

from which you see that:

$$\Big[\langle \partial_{R_\alpha}\psi_{n\mathbf{k}}|\partial_{R_\beta}\psi_{n\mathbf{k}}\rangle - \langle \partial_{R_\beta}\psi_{n\mathbf{k}}|\partial_{R_\alpha}\psi_{n\mathbf{k}}\rangle\Big] = \frac{1}{\hbar^2}\Big[\langle \partial_{k_\alpha} u_{n\mathbf{k}}|\partial_{k_\beta} u_{n\mathbf{k}}\rangle - \langle \partial_{k_\beta} u_{n\mathbf{k}}|\partial_{k_\alpha} u_{n\mathbf{k}}\rangle\Big] \ .$$

So, as anticipated, the boosting $\hbar\mathbf{k} \to \hbar\mathbf{k} + \mathbf{R}(t)$ really means that derivatives with respect to $\mathbf{R}$ are equivalent to derivatives with respect to $\hbar\mathbf{k}$. Now, the second quantization way of writing Slater determinants makes it reasonably simple to conclude that if you have many independent particles, then all you have to do is to sum over them. Without going into many details, one can show that:

$$\sigma_{\alpha\beta} = -\frac{e^2}{\hbar}\frac{1}{\text{Vol}}\sum_{\mathbf{k}}^{\text{BZ}}\sum_{n}^{\text{filled}} i\Big[\langle \partial_{k_\alpha} u_{n\mathbf{k}}|\partial_{k_\beta} u_{n\mathbf{k}}\rangle - \langle \partial_{k_\beta} u_{n\mathbf{k}}|\partial_{k_\alpha} n_{n\mathbf{k}}\rangle\Big] \ . \tag{4.50}$$

In the thermodynamic limit one can transform the sum over $\mathbf{k}$ into an integral over the BZ in the usual way. For a two-dimensional system $\frac{1}{\text{Vol}}\sum_{\mathbf{k}}^{\text{BZ}} \to \int_{\text{BZ}} \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2}$ and, recalling that $\sigma_{yx} = -\sigma_{xy}$ we can finally write:

$$\sigma_{yx} = \frac{e^2}{h}\frac{1}{2\pi}\sum_{n}^{\text{filled}} \int_{\text{BZ}} \mathrm{d}^2\mathbf{k}\ i\Big[\langle \partial_{k_x} u_{n\mathbf{k}}|\partial_{k_y} u_{n\mathbf{k}}\rangle - \langle \partial_{k_y} u_{n\mathbf{k}}|\partial_{k_x} u_{n\mathbf{k}}\rangle\Big] \ . \tag{4.51}$$

4.4. The Hall conductivity of the Haldane model

From now on we will stop denoting $\mathbf{R} = -e\mathbf{E}t$ — which was instrumental to deriving the form of the Hall conductivity in the previous section — and resume the usual meaning of $\mathbf{R}$ for the Haldane model, i.e., of an effective magnetic field for each $\mathbf{k}$, $\mathbf{R}(\mathbf{k})$. In the Haldane model, working with PBC, there are two bands, a lower band $\epsilon_{\mathbf{k}-}$ and an upper band $\epsilon_{\mathbf{k}+}$ separated by a finite gap over most of the Haldane phase diagram, i.e., away from the critical boundaries in the phase diagram in Fig. 4.3, where Dirac cones form and the system is metallic. If the number of electrons is therefore *half* the number of lattice sites — a situation commonly called as *half-filling* — then the system is a band insulator, and the lower band of energy $\epsilon_{\mathbf{k}-}$ is fully occupied. For electrons on the continuum the associated $|u_{\mathbf{k}-}\rangle$ would be a function $u_{\mathbf{k}-}(\mathbf{x})$ periodic over the unit cell of the crystal, but here we are working in tight-binding and $|u_{\mathbf{k}-}\rangle$ is simply a two-component "spinor" telling the amplitude for staying on the Wannier orbital centered on sublattice A or B in the unit cell. This identification has already been used before. So, at half-filling the spinors $|u_{\mathbf{k}-}\rangle$ constitute a completely filled band, while $|u_{\mathbf{k}+}\rangle$ is an empty band. Hence:

$$\sigma_{yx} \;=\; i\frac{e^2}{h}\frac{1}{2\pi}\int_{\mathrm{BZ}} d^2\mathbf{k}\,\Big[\langle\partial_{k_x}u_{\mathbf{k}-}|\partial_{k_y}u_{\mathbf{k}-}\rangle - \langle\partial_{k_y}u_{\mathbf{k}-}|\partial_{k_x}u_{\mathbf{k}-}\rangle\Big]\,. \tag{4.52}$$

Two observations are in order. The object we have obtained looks like an antisymmetric form closely reminiscent of a Berry curvature integrated over the whole BZ. We will see soon that indeed it is a Berry curvature form of the spin-1/2 problem, *pulled back* into $\mathbf{k}$-space by the map $\mathbf{k} \to \mathbf{R}(\mathbf{k})$ (more about this below). Second (we stress again): the σ_{yx} just calculated in this way looks pretty much as a *bulk property*: we have used PBC and even taken the thermodynamic limit. There is no trace anywhere of the *edges* of our system, to which an experimentalist would attach contacts and leads to measure currents and voltages. More comments on this bulk-edge duality in a while.

The $|u_{\mathbf{k}-}\rangle$ appearing in Eq. (4.52) must be viewed as a composite function $|u_{\mathbf{k}-}\rangle = |u_-(\mathbf{R}(\mathbf{k}))\rangle$, where $|u_-(\mathbf{R})\rangle$ is the "down spin" state when the magnetic field is in the direction of $\mathbf{R}$. Simple algebra of change of variables shows that:

$$\Big[\langle\partial_{k_x}u_{\mathbf{k}-}|\partial_{k_y}u_{\mathbf{k}-}\rangle - \langle\partial_{k_y}u_{\mathbf{k}-}|\partial_{k_x}u_{\mathbf{k}-}\rangle\Big] = \sum_{ij}\langle\partial_{R_i}u_-(\mathbf{R}))|\partial_{R_j}u_-(\mathbf{R}))\rangle\Big|_{\mathbf{R}=\mathbf{R}(\mathbf{k})} J_{ij}(\mathbf{k})\,,$$

where the Jacobian

$$J_{ij}(\mathbf{k}) = \det\begin{bmatrix}\partial_{k_x}R_i & \partial_{k_y}R_i\\ \partial_{k_x}R_j & \partial_{k_y}R_j\end{bmatrix}_{\mathbf{k}}\,, \tag{4.53}$$

appears. But $J_{ij} = -J_{ji}$ and therefore you immediately deduce that:

$$i\Big[\langle\partial_{k_x}u_{\mathbf{k}-}|\partial_{k_y}u_{\mathbf{k}-}\rangle - \langle\partial_{k_y}u_{\mathbf{k}-}|\partial_{k_x}u_{\mathbf{k}-}\rangle\Big] = \sum_{i<j}\mathcal{F}_{ij}(\mathbf{R}(\mathbf{k}))\;J_{ij}(\mathbf{k})\,,$$

in terms of the Berry curvature of a spin-1/2 problem:

$$\mathcal{F}_{ij}(\mathbf{R}) = i\left[\langle\partial_{R_i}u_-(\mathbf{R})|\partial_{R_j}u_-(\mathbf{R})\rangle - \langle\partial_{R_j}u_-(\mathbf{R})|\partial_{R_i}u_-(\mathbf{R})\rangle\right] \;=\; \epsilon^{ijk}\,\frac{R_k}{2|\mathbf{R}|^3}\,, \tag{4.54}$$

where we have introduced the totally antisymmetric tensor ϵ^{ijk} and adopted the convention of summing over repeated indices. This in turn implies that the Hall conductivity σ_{yx} of the Haldane model can be finally expressed as:

$$\sigma_{yx} = \frac{e^2}{h} \underbrace{\frac{1}{2\pi} \int_{\mathrm{BZ}} \sum_{i<j} \mathcal{F}_{ij}(\mathbf{R}(\mathbf{k}))\, J_{ij}(\mathbf{k})\, dk_x dk_y}_{c_1} = \frac{e^2}{h} c_1 \,. \tag{4.55}$$

The quantity c_1 appearing is known as *first Chern number*. It is simply the integral of the Berry curvature of the whole surface spanned by $\mathbf{R}(\mathbf{k})$, the Haldane's spaceship. You can explicitly write it as:

$$c_1 = \frac{1}{2\pi} \int_{\mathrm{BZ}} \sum_{i<j} \mathcal{F}_{ij}(\mathbf{R}(\mathbf{k}))\, J_{ij}(\mathbf{k})\, dk_x dk_y = \frac{1}{4\pi} \int_{\mathrm{BZ}} \frac{1}{|\mathbf{R}|^3}\, \mathbf{R} \cdot \left(\frac{\partial \mathbf{R}}{\partial k_x} \times \frac{\partial \mathbf{R}}{\partial k_y} \right) dk_x dk_y \,. \tag{4.56}$$

What is really crucial is that this object is *topological* in nature, i.e., it must be an integer: in the Haldane model case c_1 can be 0, 1 or -1. But adding an appropriate *third neighbor* hopping term t_3, which modifies $R_x(\mathbf{k})$ and $R_y(\mathbf{k})$, one can also obtain regions of the phase diagram where $c_1 = \pm 2$ [16, 17].

Here, let us try to guess the result. Fig. 4.5 shows, for instance, how the closed surface $\mathbf{R}(\mathbf{k})$ looks like when $\mathbf{k} \in$ BZ at two points in the phase diagram: a trivial insulator point (top and bottom-left figures, notice the origin $\mathbf{R}^* = \mathbf{0}$ outside the surface), and a topological insulator point (bottom-right figure, notice the origin $\mathbf{R}^* = \mathbf{0}$ inside the surface), both obtained for $\phi = \pi/2$. Suppose that the Haldane's spaceship $\mathbf{R}(\mathbf{k})$ lies all away and *outside* from the origin $\mathbf{R}^* = \mathbf{0}$ of the monopole field. Then you expect that the total Berry flux through this closed surface outside the singularity is exactly 0, and you would be right: $c_1 = 0$ in that case. When the Haldane's spaceship *encloses* the singularity at $\mathbf{R}^* = \mathbf{0}$, see bottom-right part of Fig. 4.5, then the solid angle through which the Berry flux goes is 4π, but the monopole "charge" is $1/2$, and there is an extra factor $1/(2\pi)$ in the definition of c_1: therefore you expect $c_1 = 1$. *Almost* right: there is a *sign* that depends on how the surface $\mathbf{R}(\mathbf{k})$ is *oriented*, which, as you know, is important in calculating fluxes. The orientation is decided by $\left(\frac{\partial \mathbf{R}}{\partial k_x} \times \frac{\partial \mathbf{R}}{\partial k_y} \right)$, and points *outward* for $\phi > 0$, in which case $c_1 = +1$, and *inward* for $\phi < 0$, $c_1 = -1$, as illustrated in Fig. 4.6

It is perhaps worth summarizing the story, from the mathematical side, like this. You have the BZ of the system, which is a torus — a closed two-dimensional surface — and $\mathbf{k}$ lives in it, $\mathbf{k} \in$ BZ. Then you have a mapping $\mathbf{k} \to \mathbf{R}(\mathbf{k})$ from the torus to $\mathbb{R}^3$, which defines a closed two-dimensional surface $\mathbf{R}(\mathbf{k})$ in $\mathbb{R}^3$: there is nothing particularly special or tricky about this mapping. But then, for each value of $\mathbf{R}(\mathbf{k})$ you have a *spinor* $|u_-(\mathbf{R})\rangle$ leaving in the two-dimensional Hilbert space $\mathbb{C}^2$: the spinor really wants to know about the direction $\hat{\mathbf{R}}$ of the field $\mathbf{R}$ — a point on the two-dimensional spin Bloch sphere $\mathbb{S}^2$ parameterized by the spherical angles θ and ϕ (not to be confused with the Haldane flux) — and you know from the discussion on the Dirac monopole that it is impossible to make a perfectly smooth choice of phase for $|u_-(\mathbf{R})\rangle$ valid over the *whole* sphere. So, the highly non-trivial issue is if the mapping

$$\mathbf{k} \to \mathbf{R} \to \hat{\mathbf{R}} = \frac{\mathbf{R}}{|\mathbf{R}|}$$

is such that the system is forced to visit the whole sphere, or only a portion of it. If $\hat{\mathbf{R}}$ visits the whole sphere as $\mathbf{k}$ runs over the BZ, it must necessarily encounter a vortex singularity

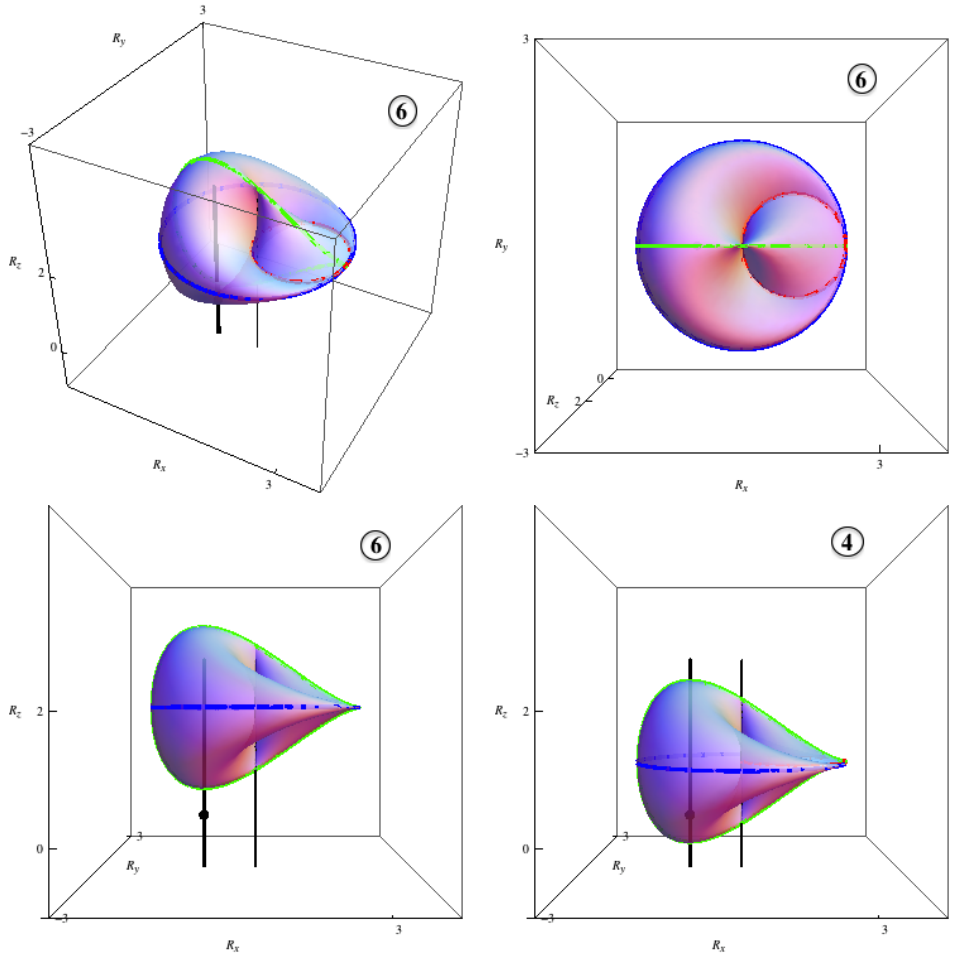

Figure 4.5.: The Haldane spaceship $\mathbf{R}(\mathbf{k})$ when $\mathbf{k}$ spans the BZ, for $\phi = \pi/2$ in the trivial (top, bottom left) and topological (bottom right) insulator region. Labels refer to the points marked in the phase diagram of Fig. 4.3.

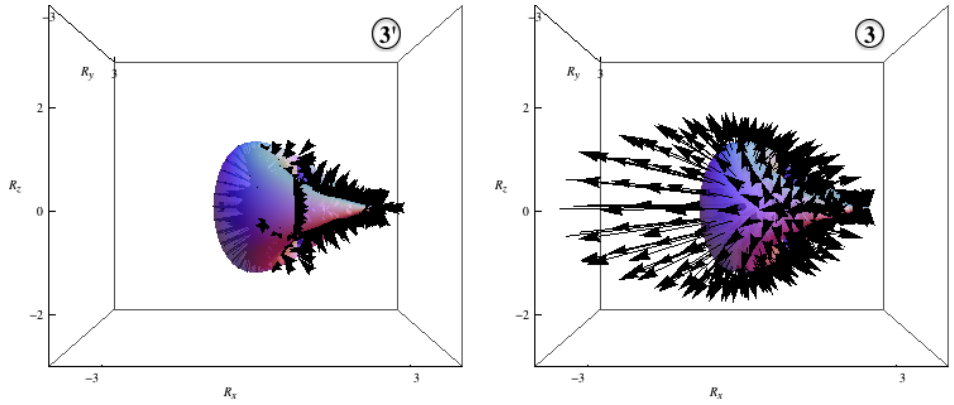

Figure 4.6.: The Haldane spaceship $\mathbf{R}(\mathbf{k})$ when $\mathbf{k}$ spans the BZ, with the orientation vectors explicitly shown: on the left $\phi = -\pi/2$, on the right $\phi = +\pi/2$. Both have $M = 0$, and are therefore in the topological insulator region (the origin is concealed inside the spaceship). Labels refer to the points marked in the phase diagram of Fig. 4.3.

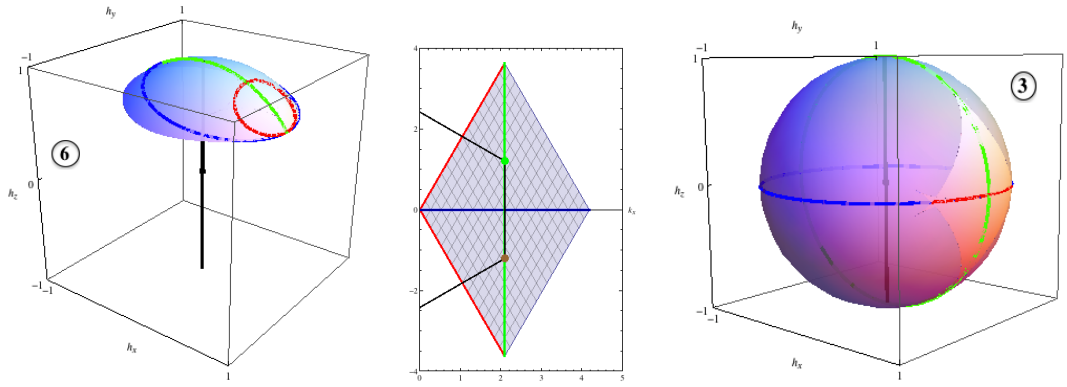

Figure 4.7.: Center: the rhombic BZ with lines running over the torus at certain special directions. Left and right: the corresponding regions of the Bloch spin sphere $\hat{\mathbf{R}}(\mathbf{k})$ generated at a trivial (left, point 6 of previous figures) or topological (right, point 3) insulator point. The color codes of the lines refer to those indicated in the central panel. Notice in particular the green line going through the Dirac points $\mathbf{K}_{\pm}$, which in the topological case runs along a full meridian of the sphere, visiting the North pole at $\mathbf{K}_{+}$ and the South pole at $\mathbf{K}_{-}$.

of the phase, otherwise not. Fig. 4.7 summarizes my effort to try to highlight the trivial vs. non-trivial nature of the mapping on the spin directions sphere.

4.5. The Haldane model on a strip: edge states

Until now we have worked with PBC and calculated the Hall conductance as a bulk property. Let us see what happens if we imagine that the model really is defined on a finite strip in the $\hat{\mathbf{x}}$-direction, while in principle infinite in the $\hat{\mathbf{y}}$-direction (or rather, wrapped on a very large cylinder).

Let me label the sites $\mathbf{r}_{j_x,j_y}$ with two integers $j_x = 1, \cdots, N_x$ and $j_y = 1, \cdots, N_y$, in the way I show (for $N_x = 10$) in Fig. 4.8. As you see from the Figure, the zig-zag lines of constant j_y run through the strip not quite along the $\hat{\mathbf{x}}$-direction, but rather at an overall angle of $\pi/3$ with the x-axis: the reason for this choice will be understood in a while. The lattice constant separating two nearby zig-zag lines, along the $\hat{\mathbf{y}}$-direction, is simply a, and the length of the whole strip along y is $L_y = N_y a$. Along the $\hat{\mathbf{y}}$-direction I assume PBC, i.e., $\hat{c}_{j_x,N_y+1} \equiv \hat{c}_{j_x,1}$ anywhere in the Hamiltonian. If the system is actually translationally invariant along y (as it is, in absence of disorder), the value of N_y will simply be a finite-size discretization of the k_y-vectors that I will introduce in a short while, but I can easily take $N_y \to \infty$ without much difficulty. Indeed, it is expedient to imagine that the PBC along y are actually realized by a "Laughlin" cylinder geometry, i.e., the strip wraps-up along the $\hat{y}$-direction into a cylinder of radius $L_y/(2\pi)$ with the cylinder-axis lying along the $\hat{\mathbf{x}}$-direction, as sketched in the right part of Fig. 4.8. This cylinder is also pierced at the center, along its $\hat{\mathbf{x}}$-axis, by an inaccessible magnetic flux Φ_y — not to be confused with the physical flux going *through* each plaquette of the strip, discussed before —, realized for instance by an infinitely long and thin solenoid.

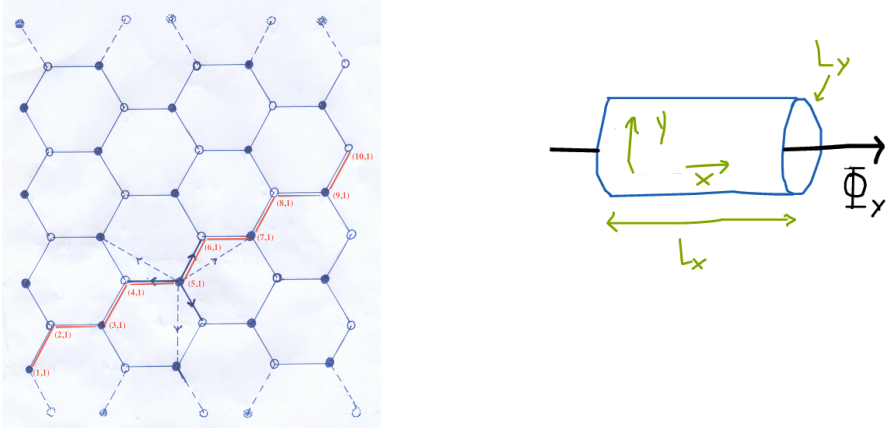

Figure 4.8.: Left: The honeycomb lattice on a finite zig-zag strip. In red I show the numbering (j_x, j_y) for the $j_y = 1$ zig-zag line discussed in the text. Right: The Laughlin cylinder geometry with the inaccessible flux piercing the cylinder.

The extra flux, which will prove immensely useful in a short while (just wait and see) can be modeled by a constant-in-space vector potential pointing along $\hat{\mathbf{y}}$, call it A_y, such that $A_y L_y = \Phi_y$, and leads to an extra Peierls's phase factor for all bonds having some component along $\hat{\mathbf{y}}$. This extra phase factor amounts to simply replacing:

$$h_{\mathbf{r}',\mathbf{r}} \to h^{\Phi_y}_{\mathbf{r}',\mathbf{r}} = \mathrm{e}^{-i(e/\hbar c)\int_{\mathbf{r}}^{\mathbf{r}'} A_y \hat{\mathbf{y}}\cdot d\mathbf{l}}\, h_{\mathbf{r}',\mathbf{r}} = \mathrm{e}^{-i\kappa_y \hat{\mathbf{y}}\cdot(\mathbf{r}'-\mathbf{r})}\, h_{\mathbf{r}',\mathbf{r}}\ , \tag{4.57}$$

where:

$$\kappa_y = \frac{2\pi}{L_y}\frac{\Phi_y}{\phi_0}\ . \tag{4.58}$$

This should appear as a kind of *déjà vu*: it is somewhat similar to the electric-field related $\mathbf{R}(t) = \hbar\boldsymbol{\kappa}(t)$ of section 4.3, except that now it has only the y component, and — at least for the time being — is not time dependent. These similarities should not obscure the fact that the geometry of the two settings and the physical interpretation of the fields present are a bit different. [22] If you go back to Eq. (4.17) expressing the tight-binding prescription for the current on a given bond, you realize (neglecting spin indices) that:

$$\hat{\mathbf{y}}\cdot\hat{\mathbf{j}}_{\mathbf{r}',\mathbf{r}} = -\frac{i}{\hbar}\hat{\mathbf{y}}\cdot(\mathbf{r}'-\mathbf{r})\left[h^{\Phi_y}_{\mathbf{r}',\mathbf{r}}\hat{c}^\dagger_{\mathbf{r}'}\hat{c}_{\mathbf{r}} - H.c.\right] = \frac{1}{\hbar}\frac{\partial}{\partial\kappa_y}\left[h^{\Phi_y}_{\mathbf{r}',\mathbf{r}}\hat{c}^\dagger_{\mathbf{r}'}\hat{c}_{\mathbf{r}} + H.c.\right]\ . \tag{4.59}$$

Summing over all bonds we realize that the *total current* along the $\hat{\mathbf{y}}$-direction can be simply written as:

[22] In section 4.3 we had a planar two-dimensional geometry and $\mathbf{R}(t)$ — necessarily time-dependent — was associated to a small uniform electric field, but no extra magnetic field whatsoever was present, and no notion of an associated flux quantum. Here, the geometry is that of a cylinder, and there is a magnetic flux Φ_y on the cylinder axis, but no electric field whatsoever, *unless* Φ_y is made time-dependent, as we shall indeed do in discussing Laughlin's argument. A time-dependent magnetic flux $\Phi_y(t)$ varying linearly with t will indeed generate, by Faraday's law, an axial constant-in-time electric field which appears uniform and along $\hat{\mathbf{y}}$ if looked on the surface of the cylinder.

$$\hat{J}_y = \hat{\mathbf{y}} \cdot \widehat{\mathbf{J}} = \frac{1}{\hbar} \frac{\partial}{\partial \kappa_y} \hat{H}(\kappa_y) \; . \tag{4.60}$$

Notice that this equality holds true even in presence of *disorder* — where I *cannot* Fourier transform along y and introduce k_y-vectors, as we will do in a second — and even when you have Hubbard-like *interactions* in your tight-binding problem. If $|\Psi_0(\kappa_y)\rangle$ denotes the *ground state* of the system for a given value of κ_y, then the Hellman-Feynman theorem guarantees that you can write:

$$\langle \Psi_0(\kappa_y)|\hat{J}_y|\Psi_0(\kappa_y)\rangle = \frac{1}{\hbar}\frac{\partial}{\partial \kappa_y}\langle \Psi_0(\kappa_y)|\hat{H}(\kappa_y)|\Psi_0(\kappa_y)\rangle = \frac{1}{\hbar}\frac{\partial E_0(\kappa_y)}{\partial \kappa_y} \; . \tag{4.61}$$

So, if the total energy of the system *does not depend* on the inaccessible flux Φ_y, then there must be no total current in the ground state. If you recall that the (space-averaged) electronic current density is:

$$j_y^e = -e \frac{\langle \Psi_0(0)|\hat{J}_y|\Psi_0(0)\rangle}{L_x L_y} \; ,$$

the total current flowing along the strip is $I_y = L_x j_y^e$, and $\kappa_y = \frac{2\pi}{L_y}\frac{\Phi_y}{\phi_0}$, see Eq. (4.58), then you can equivalently recast the previous expression in the following form:

$$I_y = -\frac{e}{\hbar L_y}\frac{\partial E_0(\kappa_y)}{\partial \kappa_y}\Big|_{\kappa_y=0} = -c\frac{\partial E_0(\Phi_y)}{\partial \Phi_y}\Big|_{\Phi_y=0} \; . \tag{4.62}$$

A totally equivalent way of seeing the inaccessible flux Φ_y is that you have *twisted* the boundary conditions along the y direction. Indeed, you can actually *eliminate* the appearance of Φ_y anywhere in the Hamiltonian if you make a canonical transformation

$$\hat{c}_{j_x,j_y} \to \tilde{c}_{j_x,j_y} = \mathrm{e}^{i\kappa_y \hat{\mathbf{y}}\cdot \mathbf{r}_{j_x,j_y}} \; \hat{c}_{j_x,j_y} \; , \tag{4.63}$$

as a simple calculation will show: remember that, after all, we are dealing with a constant-in-space vector potential A_y which you can eliminate by a gauge transformation of the phase. And indeed, if the system had *open boundary conditions* along the $\hat{\mathbf{y}}$-direction, as we are assuming for the $\hat{\mathbf{x}}$-direction, then you might eliminate the effect of the flux Φ_y leaving no trace of it. **But**, if you really have PBC (i.e., the system lives on a cylinder) then eliminating the presence of Φ_y in all internal bonds thorough the canonical transformation in Eq. (4.63) will inevitably lead to a *twist* of the boundary condition along $\hat{\mathbf{y}}$. Indeed, before the canonical transformation we had PBC, i.e., $\hat{c}_{j_x,N_y+1} \equiv \hat{c}_{j_x,1}$, but now:

$$\tilde{c}_{j_x,N_y+1} = \mathrm{e}^{i\kappa_y a(N_y+1)} \; \hat{c}_{j_x,N_y+1} = \mathrm{e}^{i\kappa_y L_y}\mathrm{e}^{i\kappa_y a} \; \hat{c}_{j_x,1} = \mathrm{e}^{i2\pi\frac{\Phi_y}{\phi_0}} \; \tilde{c}_{j_x,1} \; , \tag{4.64}$$

a relationships that defines more general *twisted boundary conditions* along $\hat{\mathbf{y}}$, unless the inaccessible flux Φ_y is a multiple of the flux quantum ϕ_0, in which case the canonical transformation (4.63) completely eliminates Φ_y, still retaining PBC. More about currents and fluxes in a while.

Let us get back to our Haldane strip geometry, and change, accordingly, notation from $\hat{c}_{\mathbf{r}} \to \hat{c}_{j_x,j_y}$. I assume that the atom with $j_x = 1$ belongs to the A-sublattice. Since the

problem (in absence of disorder) is translationally invariant along $\hat{\mathbf{y}}$, we introduce a Fourier transform of the operators along $\hat{\mathbf{y}}$:

$$\hat{c}^\dagger_{j_x,k_y} = \frac{1}{\sqrt{N_y}} \sum_{j_y=1}^{N_y} \mathrm{e}^{iak_y j_y} \hat{c}^\dagger_{j_x,j_y} \qquad \text{and} \qquad \hat{c}^\dagger_{j_x,j_y} = \frac{1}{\sqrt{N_y}} \sum_{k_y}^{\mathrm{BZ_y}} \mathrm{e}^{-iak_y j_y} \hat{c}^\dagger_{j_x,k_y} \ , \tag{4.65}$$

Inserting this expression for $\hat{c}_{j_x,j_y}$ in the Hamiltonian and using translational invariance along y one arrives at the following form:

$$\hat{H}_{\mathrm{Hal}} = \sum_{k_y}^{\mathrm{BZ_y}} \hat{H}_{k_y} \ ,$$

where, for each given wave-vector k_y, we have to diagonalize a Hamiltonian working only on the N_x operators $\hat{c}_{j_x,ky}$, along a zig-zag line. The transformation is tedious but rather straightforward. [23] We get, for each k_y, a tight-binding problem with hopping up to second-

[23] One needs to distinguish sites (j_x, j_y) with $j_x = j_o$ *odd*, from those with $j_x = j_e$ *even*. Start from $j_x = j_o$, and collect all the terms of the Hamiltonian which do not change j_o:

$$\hat{H}_{\mathrm{site},j_o} = \sum_{j_y=1}^{N_y} \left[M \hat{c}^\dagger_{j_o,j_y} \hat{c}_{j_o,j_y} + t_2 \mathrm{e}^{-i\phi} \mathrm{e}^{-ia\kappa_y} \hat{c}^\dagger_{j_o,j_y+1} \hat{c}_{j_o,j_y} + t_2 \mathrm{e}^{i\phi} \mathrm{e}^{ia\kappa_y} \hat{c}^\dagger_{j_o,j_y-1} \hat{c}_{j_o,j_y} \right] \ .$$

Upon Fourier-transforming in y we get:

$$\hat{H}_{\mathrm{site},j_o} = \sum_{k_y}^{\mathrm{BZ_y}} \underbrace{\left[M + t_2 \mathrm{e}^{-i\phi} \mathrm{e}^{-ia(k_y+\kappa_y)} + t_2 \mathrm{e}^{i\phi} \mathrm{e}^{ia(k_y+\kappa_y)} \right]}_{\epsilon_{j_o}(k_y)} \hat{c}^\dagger_{j_o,k_y} \hat{c}_{j_o,k_y} \ .$$

Similarly, for the nearest-neighbor terms:

$$\begin{aligned} \hat{H}_{\mathrm{nn},j_o} &= \sum_{j_y=1}^{N_y} \left[t_1 \mathrm{e}^{-ia\kappa_y/2} \hat{c}^\dagger_{j_o+1,j_y} \hat{c}_{j_o,j_y} + t_1 \mathrm{e}^{ia\kappa_y/2} \hat{c}^\dagger_{j_o+1,j_y} \hat{c}_{j_o,j_y+1} \ + \ \mathrm{H.c.} \right] \\ &= \sum_{k_y}^{\mathrm{BZ_y}} \left\{ \underbrace{\left[t_1 \mathrm{e}^{-ia\kappa_y/2} (1 + \mathrm{e}^{ia(k_y+\kappa_y)}) \right]}_{h_{j_o+1,j_o}(k_y)} \hat{c}^\dagger_{j_o+1,k_y} \hat{c}_{j_o,k_y} \ + \ \mathrm{H.c.} \right\} \ . \end{aligned}$$

Finally, for second-neighbor hoppings:

$$\begin{aligned} \hat{H}_{\mathrm{nnn},j_o} &= \sum_{j_y=1}^{N_y} \left[t_2 \mathrm{e}^{i\phi} \mathrm{e}^{-ia\kappa_y/2} \hat{c}^\dagger_{j_o+2,j_y} \hat{c}_{j_o,j_y} + t_2 \mathrm{e}^{-i\phi} \mathrm{e}^{ia\kappa_y/2} \hat{c}^\dagger_{j_o+2,j_y} \hat{c}_{j_o,j_y+1} \ + \ \mathrm{H.c.} \right] \\ &= \sum_{k_y}^{\mathrm{BZ_y}} \left\{ \underbrace{\left[t_2 \mathrm{e}^{-ia\kappa_y/2} (\mathrm{e}^{i\phi} + \mathrm{e}^{-i\phi} \mathrm{e}^{ia(k_y+\kappa_y)}) \right]}_{h_{j_o+2,j_o}(k_y)} \hat{c}^\dagger_{j_o+2,k_y} \hat{c}_{j_o,k_y} \ + \ \mathrm{H.c.} \right\} \ . \end{aligned}$$

The $j_x = j_e$ *even* cases are treated in an entirely similar way and differ just by a change $M \to -M$, $\phi \to -\phi$ and the fact that the nearest-neighbor term is now simply $h_{j_e+1,j_e} = t_1$ without any phase factor. This is the appropriate place to observe that, had I chosen as basic lines the arm-chair ones, running parallel to the x-axis, instead of the $\pi/3$-inclined zig-zag lines, then the apparent periodicity of the resulting chain would be *four* rather than *two*: obviously the two choices can be shown to be equivalent, as usual, by a unitary transformation.

neighbors of the generic form:

$$\begin{aligned}\hat{H}_{k_y} &= \sum_{j=1}^{N_x-1}\Big[h_{j+1,j}(k_y)\,\hat{c}^\dagger_{j+1,k_y}\hat{c}_{j,k_y}+\text{H.c.}\Big]+\sum_{j=1}^{N_x-2}\Big[h_{j+2,j}(k_y)\,\hat{c}^\dagger_{j+2,k_y}\hat{c}_{j,k_y}+\text{H.c.}\Big]\\ &+ \sum_{j=1}^{N_x}\epsilon_j(k_y)\,\hat{c}^\dagger_{j,k_y}\hat{c}_{j,k_y}\ ,\end{aligned} \tag{4.66}$$

where the parameters are found to be (see previous footnote for details), using the shorthand j_o and j_e for *odd* or *even* values of j:

$$\begin{cases}\epsilon_{j_o}=M+2t_2\cos\left[a(k_y+\kappa_y)+\phi\right]\\ h_{j_o+1,j_o}=t_1 e^{-ia\kappa_y/2}[1+e^{ia(k_y+\kappa_y)}]\\ h_{j_o+2,j_o}=t_2 e^{-ia\kappa_y/2}[e^{i\phi}+e^{-i\phi}e^{ia(k_y+\kappa_y)}]\end{cases}\qquad\begin{cases}\epsilon_{j_e}=-M+2t_2\cos\left[a(k_y+\kappa_y)-\phi\right]\\ h_{j_e+1,j_e}=t_1\\ h_{j_e+2,j_e}=t_2 e^{-ia\kappa_y/2}[e^{-i\phi}+e^{i\phi}e^{ia(k_y+\kappa_y)}]\end{cases}. \tag{4.67}$$

Notice how the inaccessible flux κ_y appears only in combination with k_y, apart from an overall phase-factor $e^{-ia\kappa_y/2}$ that might be eliminated by a canonical transformation. [24]

To appreciate in a simple way why **edge modes** occur for the strip, let us consider the case of graphene, that is assume $t_2 = M = 0$, i.e., the previous model with t_1 only, and put $\kappa_y = 0$: then the strip Hamiltonian has $\epsilon_j = 0$ and all second-neighbor hoppings vanish, $h_{j+2,j} = 0$. The nearest-neighbor hoppings are $h_{j_e+1,j_e} = t_1$ for the even sites, but $h_{j_o+1,j_o} = t_1[1+e^{iak_y}]$ for the odd sites. We notice that if $k_y = \pi/a$ then $h_{2,1} = 0$, i.e., the site with $j = 1$ is totally *decoupled* from the rest of the chain. If N_x is *even*, i.e., the right-end edge is again an A-site, then a similar fate occurs to the hopping $h_{N_x,N_x-1} = 0$, and the $j = N_x$-site is also decoupled. Now, for every finite N_x, there is a (small) gap in the dispersion of the graphene strip bands (i.e., strictly speaking no Dirac-cone touching of bands), and in the middle of this small gap an essentially non-dispersive band of edge modes appears. We are not going to show these results. If you are curious, see for instance Ref. [18]. Now let us consider a finite $t_2 > 0$ (we take $t_2/t_1 = 0.3$), and plot the bands obtained for a finite Haldane-model zig-zag strip at $\phi = \pi/2$ for four values of $M/t_2 = 4\sqrt{3}, 3\sqrt{3}, 2\sqrt{3}, 0$. Fig. 4.9 illustrates the result of such calculation. Notice that there are always states induced by the fact that N_x is finite (the blue dots), but the striking feature of the bottom plots in Fig. 4.9, corresponding to the two topological insulator points at $M/t_2 = 2\sqrt{3}$ (left) and $M/t_2 = 0$ (right), is that such states **1)** *cross the bulk gap*, **2)** are associated to edge states, i.e., with wave-functions exponentially localized at an edge of the strip, and **3)** they *carry a current.*

How do we make sense of these findings? One way to understand the nature of the solutions in the strip case is to write the Schrödinger equation (SE) into an equivalent *transfer matrix* (TM) form. Let us write, in first quantization form, the SE for the amplitude $\psi_{j\alpha}$ of the α-eigenstate on the strip, neglecting the label k_y, and even α, to shorten the notation. The SE is:

$$h_{j,j+2}\psi_{j+2}+h_{j,j+1}\psi_{j+1}+\epsilon_j\psi_j+h_{j,j-1}\psi_{j-1}+h_{j,j-2}\psi_{j-2}=E\psi_j$$

[24] Simply transform

$$\hat{c}_{j,k_y}\to\tilde{c}_{j,k_y}=e^{i\kappa_y\hat{\mathbf{y}}\cdot(\mathbf{r}_{j,1}-\mathbf{r}_{1,1})}\hat{c}_{j,k_y}\ ,$$

and the annoying factor will magically vanish. Here $\hat{\mathbf{y}}\cdot(\mathbf{r}_{j,1}-\mathbf{r}_{1,1})$ is simply the y-height along the zig-zag chain of the site at $j_x = j$ with respect to the left site at $j_x = 1$.

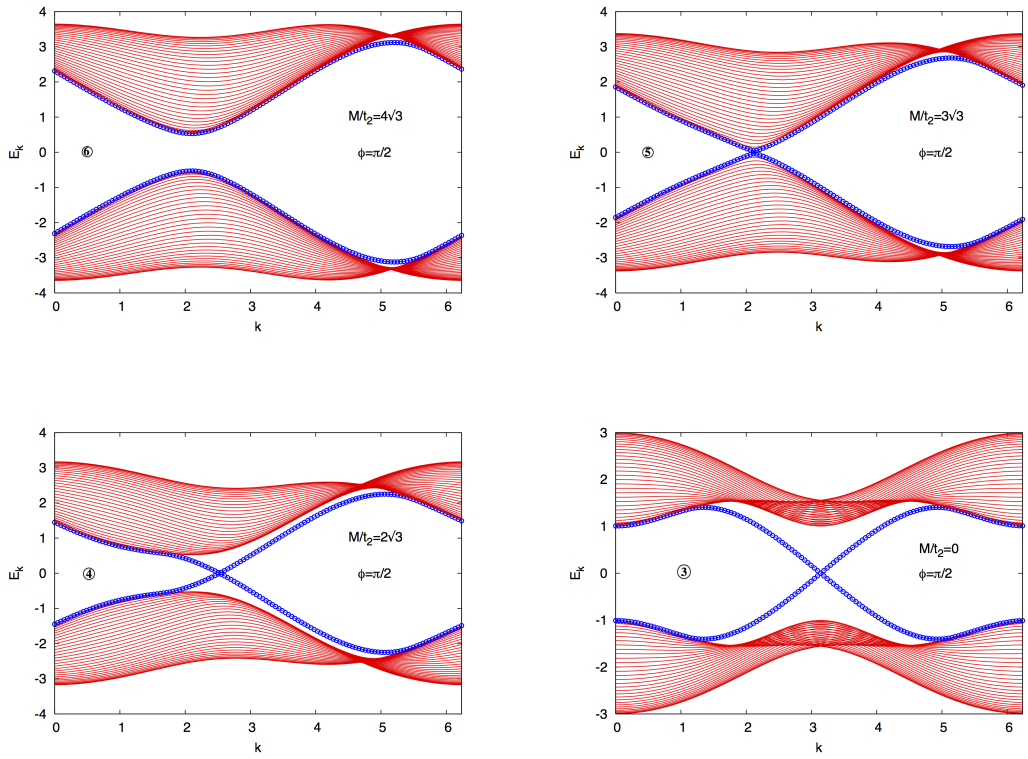

Figure 4.9.: Bands for Haldane-model zig-zag strip with $N_x = 64$, for $\phi = \pi/2$ and $M/t_2 = 4\sqrt{3}$ (top left, ordinary insulator), $M/t_2 = 3\sqrt{3}$ (top right, critical point), $M/t_2 = 2\sqrt{3}$ or $M/t_2 = 0$ (bottom, topological insulator). The blue dot curves are states associated to the finiteness of N_x, see discussion in the text. Labels refer to the points marked in the phase diagram of Fig. 4.3.

Assuming that $h_{j,j+1} \neq 0$ we can reorganize the terms in a recursive way as:

$$\psi_{j+2} = -\frac{h_{j,j+1}}{h_{j,j+2}}\psi_{j+1} + \frac{(E-\epsilon_j)}{h_{j,j+2}}\psi_j - \frac{h_{j,j-1}}{h_{j,j+2}}\psi_{j-1} - \frac{h_{j,j-2}}{h_{j,j+2}}\psi_{j-2} \ ,$$

or, equivalently, into a 4×4 matrix form, as follows:

$$\begin{pmatrix} \psi_{j+2} \\ \psi_{j+1} \\ \psi_j \\ \psi_{j-1} \end{pmatrix} = \underbrace{\begin{pmatrix} -\frac{h_{j,j-1}}{h_{j,j+2}} & \frac{(E-\epsilon_j)}{h_{j,j+2}} & -\frac{h_{j,j-1}}{h_{j,j+2}} & -\frac{h_{j,j-2}}{h_{j,j+2}} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}}_{\mathbf{T}_j} \begin{pmatrix} \psi_{j+1} \\ \psi_j \\ \psi_{j-1} \\ \psi_{j-2} \end{pmatrix} = \mathbf{T}_j \begin{pmatrix} \psi_{j+1} \\ \psi_j \\ \psi_{j-1} \\ \psi_{j-2} \end{pmatrix} . \tag{4.68}$$

The transfer matrix $\mathbf{T}_j$ has determinant $\det \mathbf{T}_j = -h_{j,j-2}/h_{j,j+2}$, as you can easily prove by expanding over the last column. You can also easily show that, given the *even/odd* alternation of the couplings, there are indeed two types of $\mathbf{T}_j$, the $\mathbf{T}_e$ and the $\mathbf{T}_o$, both having $|\det \mathbf{T}_{e/o}| = 1$. The recursive structure of the equation is simple. For $j = j_e$, for instance:

$$\begin{pmatrix} \psi_{j_e+1} \\ \psi_{j_e} \\ \psi_{j_e-1} \\ \psi_{j_e-2} \end{pmatrix} = \mathbf{T}_o \, \mathbf{T}_e \, \cdots \, \mathbf{T}_o \, \mathbf{T}_e \, \underbrace{\mathbf{T}_o \, \mathbf{T}_e}_{\mathbf{M}} \begin{pmatrix} \psi_1 \\ \psi_0 \\ \psi_{-1} \\ \psi_{-2} \end{pmatrix} , \tag{4.69}$$

where we have identified the relevant matrix $\mathbf{M} = \mathbf{T}_o\mathbf{T}_e$ which has to be applied repeatedly to advance the state. Let us know discuss boundary conditions. At the left edge of the strip, which starts at $j = 1$, we must put $\psi_0 = \psi_{-1} = \psi_{-2} = 0$. If the width of the strip is such that N_x is even we then have:

$$\begin{pmatrix} \psi_{N_x+1} \\ \psi_{N_x} \\ \psi_{N_x-1} \\ \psi_{N_x-2} \end{pmatrix} = \underbrace{\mathbf{M} \, \cdots \, \mathbf{M} \, \mathbf{M}}_{\frac{N_x}{2}\text{-terms}} \begin{pmatrix} \psi_1 \\ 0 \\ 0 \\ 0 \end{pmatrix} , \tag{4.70}$$

A few comments are here in order. First of all, we do not know the value of ψ_1: due to linearity, however, a rescaling of ψ_1 by a constant A rescales the whole wave-function by A. Eventually, such a rescaling will be used to normalize the wave-function. Next, the equations involve an energy E — hidden inside the belly of $\mathbf{M}$ — which we can set at our will: evidently, most of the choices of E will not correspond to eigenvalues of the problem. For a chain of size N_x, the N_x values of E which are eigenvalues of the SE are those for which the final value of ψ_{N_x+1} turns out to be zero (recall that we are imposing open BC on the strip). Now, ψ_{N_x+1} can be expressed as:

$$0 = \psi_{N_x+1} = \left[\mathbf{M}^{\frac{N_x}{2}}\right]_{11} \psi_1 \ , \tag{4.71}$$

which is indeed a polynomial of degree N_x in the variable E, admitting N_x solutions E_α with $\alpha = 1, \cdots, N_x$. The correct eigenvalues and associated eigenvectors are therefore only accessible by a "shooting" technique, or through the direct solution of the eigenvalue problem, both not particularly straightforward (i.e., in general one has to resort to some numerical routine). There is, however, an important property of the wave-function which we can easily understand from the recursive structure of the wave-function. Recall that $\mathbf{M}$ is a 4×4 matrix

whose determinant has modulus 1, $|\det \mathbf{M}| = 1$. If you denote by μ_β the 4 eigenvalues if $\mathbf{M}$, the $|\det \mathbf{M}| = \prod_{\beta=1}^{4} |\mu_\beta| = 1$. There are now essentially two possibilities: *(i)* the eigenvalues μ_β are all on the unit circle, $|\mu_\beta| = 1$, or *(ii)* there are *pairs* of eigenvalues such that $\mu_\pm = \mathrm{e}^{\pm\lambda} w_\pm$, with $|w_\pm| = 1$. Now consider what happens to an arbitrary vector $\mathbf{v}_0 = (\psi_1, 0, 0, 0)^T$ when we apply to it j times the matrix $\mathbf{M}$, i.e., $\mathbf{v}_j = \mathbf{M}^j \mathbf{v}_0$. If we expand the initial vector $\mathbf{v}_0$ on the basis of the eigenvectors of $\mathbf{M}$, $\mathbf{v}_\beta$, $\mathbf{v}_0 = \sum_\beta a_\beta \mathbf{v}_\beta$, we have that $\mathbf{v}_j = \sum_\beta a_\beta \mu_\beta^j \mathbf{v}_\beta$. In case *(ii)*, corresponding to energies E outside the bulk energy spectrum of the problem, the component of $\mathbf{v}_j$ proportional to the eigenvector $\mathbf{v}_+$ with eigenvalue $\mu_+ = e^\lambda w_+$ is amplified at every iteration, so that the norm of $\mathbf{v}_j$ explodes exponentially, $\|\mathbf{v}_j\|^2 \approx \|a_+ e^{\lambda j} \mathbf{v}_+\|^2 = |a_+|^2 e^{2\lambda j}$, unless the initial vector $\mathbf{v}_0$ is chosen in such a way that $a_+ \equiv 0$. One can show that, in this case, the correct solution is indeed exponentially decreasing with increasing j. On the contrary, in case *(i)* — corresponding to energies E inside the allowed bulk spectral range — all components are simply multiplied by phases, and the norm of the vector is not exponentially amplified. These are the ordinary "bulk" plane-wave-like Bloch states. If you are interested in this type of analysis of the TM approach, although in a simpler setting, please refer to the detailed discussion given in the book by Bernevig [18].

Let us continue now our discussion with an analysis of the results that you find by numerically solving the SE problem without any TM. The fact that the bands crossing the gap are associated to edge states is clarified by Fig. 4.10, showing the exponentially localized wavefunctions for the states just before the crossing point k_c, at $k_y = k_c - 2\pi/L_y$ (left panel), and just after k_c, at $k_y = k_c + 2\pi/L_y$ (right panel). This exponential localization of the states is

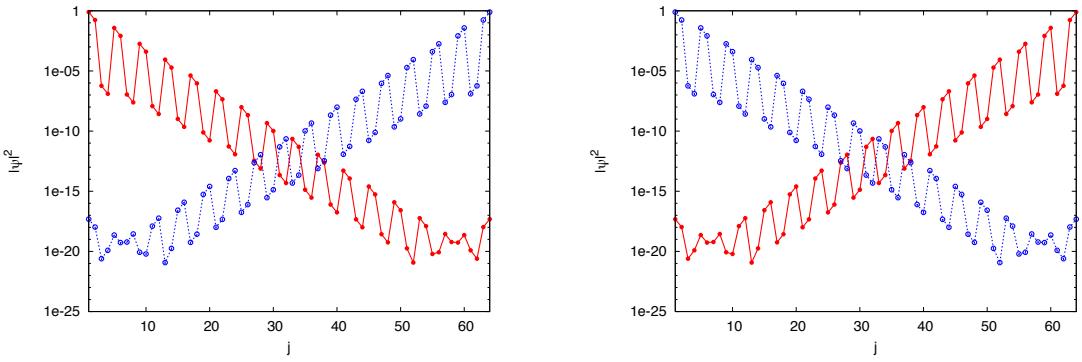

Figure 4.10.: $|\psi|^2$ of edge states, for $M = 0$ and $\phi = \pi/2$, at $k_y = k_c - 2\pi/L_y$ (left), and $k_y = k_c + 2\pi/L_y$ (right), where $k_c = \pi/a$ is the "crossing" point of the edge bands. In both panels, red curves are associated to the lower-in-energy edge-state for each k_y, blue curves to the higher-in-energy edge-state.

actually there only for the k_y points where the edge-bands are sufficiently far away from the other bulk bands. For $k_y = 0$, for instance, that would not be true: the blue-dotted bands are actually associated to bulk states in such cases, as you can see from Fig. 4.11 where the wave-function of the state with $k_y = 0$ is shown. A peculiar fact also occurs for $k_y = k_c$: there you would think that the two edge bands actually *cross*, but you can show that in reality they never actually cross, because there is an extremely small but finite *gap* which leads in

the end to an *avoided crossing*: we will discuss this point further below, in due time; for the time being, just be aware that this is simply the tiny gap accompanying the fact that the lower energy state is actually symmetrically living on the left and right edge, while the higher energy state is the corresponding anti-symmetric combination, just as you get in a double well.

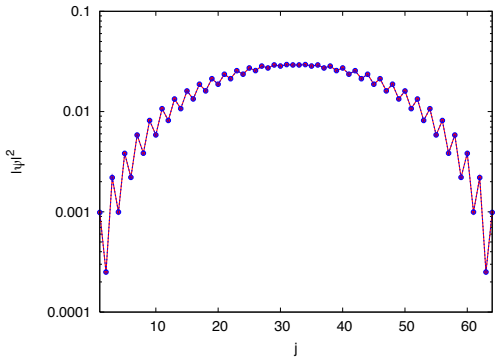

Figure 4.11.: $|\psi|^2$ of the state at $k_y = 0$, i.e., at the "top" of the valence band, showing that this is actually a bulk state.

To appreciate the question of the current carried by each state, let us go back to our strip problem in Eq. (4.66). For any fixed value of k_y, the strip Hamiltonian is a specific case of general quadratic form:

$$\hat{H}_{k_y} = \sum_{j'j} h_{j'j}(k_y)\, \hat{c}^\dagger_{j',k_y} \hat{c}_{j,k_y} \ , \tag{4.72}$$

where $h_{j'j} = h^*_{jj'}$ (i.e., $\mathbf{h} = \mathbf{h}^\dagger$ is Hermitean). Suppose that we diagonalize $\hat{H}_{k_y}$ and find for every k_y its eigenstates $\psi_{j\alpha}$ — which we know denote by $u_{j\alpha}(k_y)$ — with associated eigenvalues $E_\alpha(k_y)$. The eigenstates $u_{j\alpha}(k_y)$ can be regarded as the columns of an $N_x \times N_x$ unitary matrix $\mathbf{U}_{k_y}$, with increasing energy as the column index $\alpha = 1 \cdots N_x$ increases. The operator $\hat{a}^\dagger_{\alpha k_y}$ associated to the α-th eigenstate at fixed k_y is: [25]

$$\hat{a}^\dagger_{\alpha k_y} = \sum_j u_{j\alpha}(k_y) \hat{c}^\dagger_{j,k_y} = \sum_j \left[\mathbf{U}^T_{k_y}\right]_{\alpha j} \hat{c}^\dagger_{j,k_y} \ .$$

The bands displayed in Fig. 4.9 are nothing but the N_x energy eigenvalues $E_{\alpha=1\cdots N_x}(k_y)$ versus k_y.

Let us consider the problem of determining the current carried by each single-particle eigenstate: since we are dealing with a independent-particle problem, the current of a Slater determinant of two or more particles $\hat{a}^\dagger_{\alpha k_y}$ is simply the sum of the currents carried by each single particle. In turn the current of each single particle can be determined by the following

[25] In matrix form, this can be written as

$$\hat{\mathbf{a}}^\dagger_{k_y} = \mathbf{U}^T_{k_y} \cdot \hat{\mathbf{c}}^\dagger_{k_y} \qquad \Rightarrow \qquad \hat{\mathbf{c}}_{k_y} = \mathbf{U}_{k_y} \cdot \hat{\mathbf{a}}_{k_y} \ . \tag{4.73}$$

trick. Consider the single-particle state $\hat{a}^\dagger_{\alpha k_y}|0\rangle \to |\Psi_\alpha(\kappa_y)\rangle$ and apply to it the Hellman-Feynman's relationship in Eq. (4.61). Recalling that everything depends on κ_y in exactly the same way as it depends on k_y, we can easily write:

$$\langle\Psi_\alpha(\kappa_y)|\hat{J}_y|\Psi_\alpha(\kappa_y)\rangle = \frac{1}{\hbar}\frac{\partial}{\partial\kappa_y}\langle\Psi_\alpha(\kappa_y)|\hat{H}(\kappa_y)|\Psi_\alpha(\kappa_y)\rangle = \frac{1}{\hbar}\frac{\partial E_\alpha(k_y)}{\partial k_y}\,, \tag{4.74}$$

i.e., the current carried by each single-particle state $\hat{a}^\dagger_{\alpha k_y}$ can be easily read-off from the *slope* of the corresponding dispersion $E_\alpha(k_y)$. Now suppose that the number of particles with which we form our Slater determinant is such the system is exactly half-filled, $N = N_x N_y/2$. Each full band can hold N_y particles, one for each of the N_y k_y-points (recall that there is no spin here, so that Pauli principle allows only one particle per site). The bands shown as red solid lines — lying below the blue-dotted gap-crossing states — are then all completely filled with particles, while the gap-crossing states are only filled *below* the Fermi energy, passing through the crossing point k_c. Each completely filled band carries no total current, as you can simply show:

$$\langle\Psi_\alpha|\hat{J}_y|\Psi_\alpha\rangle = \sum_{k_y}^{\rm BZ}\frac{1}{\hbar}\frac{\partial E_\alpha(k_y)}{\partial k_y} \to L\int_0^{2\pi}\frac{{\rm d}k}{2\pi}\,\frac{1}{\hbar}\frac{\partial E_\alpha(k)}{\partial k} = 0\,,$$

where now $|\Psi_\alpha\rangle = \prod_{k_y}^{\rm BZ}\hat{a}^\dagger_{\alpha k_y}|0\rangle$ denotes the Slater determinant with the filled α-band, and the result follows because $E_\alpha(k)$ is a periodic function over the BZ.

Now consider the two edge-states bands. Again, call k_c the k_y-point where the two bands cross (where $k_c = \pi/a$ for $M = 0$ and $\phi = \pi/2$, but is in general different from π/a for $M \neq 0$ and/or $\phi \neq \pi/2$). All the edge states with energy below the Fermi energy, going through the "crossing" point, are filled: call this band $E_{{\rm edge},-}(k_y)$ (notice it has a singular derivative at k_c), while the states above the crossing point — with energy $E_{{\rm edge},+}(k_y)$ —are empty. The occupied states of $E_{{\rm edge},-}(k_y)$ with $k_y < k_c$ tend to carry a *positive current*, mostly through the edge states localized at the *left edge*, while those with $k_y > k_c$ tend to carry a *negative current*, mostly through the edge states localized at the *right edge*. However, by splitting the current integral at k_c, where $\frac{\partial E_{{\rm edge},-}(k_y)}{\partial k_y}$ abruptly switches from positive to negative, you can easily convince yourself that the total current carried by the edge states still vanishes:

$$\begin{aligned}\langle\Psi_{{\rm edge},-}|\hat{J}_y|\Psi_{{\rm edge},-}\rangle \;&\to\; L\Big[\int_0^{k_c} + \int_{k_c}^{2\pi}\Big]\frac{{\rm d}k}{2\pi}\,\frac{1}{\hbar}\frac{\partial E_{{\rm edge},-}(k_y)}{\partial k_y}\\ &=\; \frac{L}{2\pi\hbar}\Big([E_{{\rm edge},-}(k_c) - E_{{\rm edge},-}(0)] + [E_{{\rm edge},-}(\frac{2\pi}{a}) - E_{{\rm edge},-}(k_c)]\Big) = 0\,,\end{aligned}$$

where again the result follows from the fact that $E_{{\rm edge},-}(2\pi/a) = E_{{\rm edge},-}(0)$. In essence, the overall positive current carried at the left edge is exactly compensated by an overall negative current at the right edge, and no net current flows in the $\hat{\mathbf{y}}$-direction.

You should not be surprised by this result. It is evident that the system, in the topologically non-trivial phase, has microscopic currents going on at the edges, but there cannot be an overall current in the $\hat{\mathbf{y}}$ direction unless you break the symmetry in some way, for instance by putting a voltage V_x across the strip! We will show this explicitly in the next section.

4.6. The strip in presence of an applied voltage

Suppose you now apply a uniform and constant electric field E_x along the $\hat{\mathbf{x}}$-direction, in which the strip is finite. You can conveniently represent this in the scalar potential gauge, i.e., you apply a voltage bias V_x across the strip; this does no harm, since translational invariance cannot be used anyway along $\hat{\mathbf{x}}$. The Haldane model is then supplemented by an extra scalar potential term of the form:

$$\hat{H}_{V_x} = -\frac{eV_x}{L_x} \sum_{\mathbf{r}} (\hat{\mathbf{x}} \cdot \mathbf{r})\, \hat{n}_{\mathbf{r}} \,, \tag{4.75}$$

corresponding to a uniform electric field $\mathbf{E} = -\hat{\mathbf{x}} V_x / L_x$. We will take in the following $V_x < 0$ so that the electric field is in the positive $\hat{\mathbf{x}}$-direction, and assume that the origin $\mathbf{r} = \mathbf{0}$ coincides with the A-site labeled by $j_x = j_y = 1$ in Fig. 4.8. Fig. 4.12 shows the dispersion

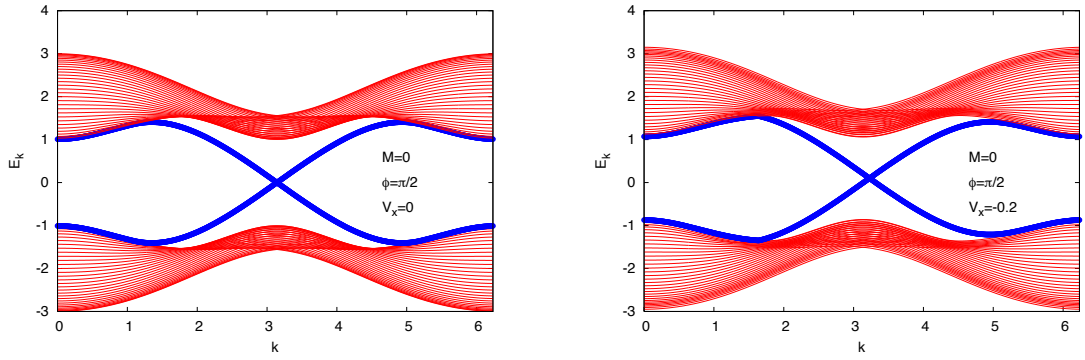

Figure 4.12.: Edge states for the Haldane model with $M = 0$ and $\phi = \pi/2$, at $V_x = 0$ (left) and $V_x/t_1 = -0.2$ (right). The differences are hardly noticeable on this scale. See below for a closer view and comparison.

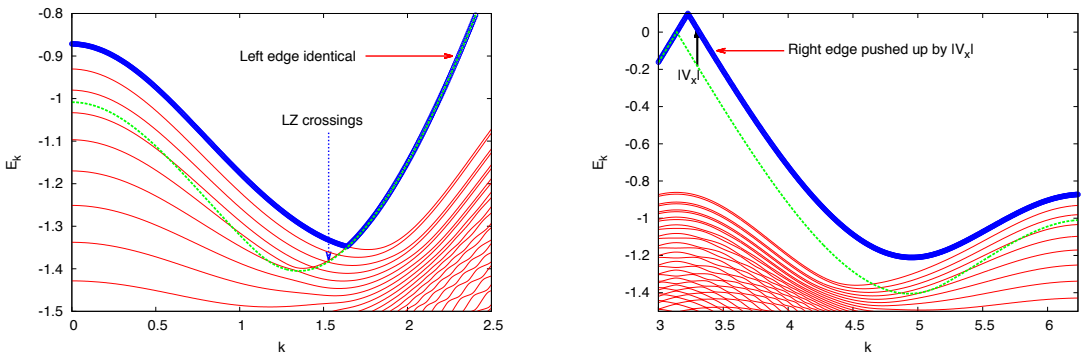

Figure 4.13.: A zoom on the structure of the bands for $V_x/t_1 = -0.2$ close to $k_y = 0$ (left) and $k_y = 2\pi/a$ (right), compared with the $V_x = 0$ edge bands, shown as dashed lines. Notice how the left edge state is unaffected by V_x, while the right edge state energy is pushed up by $|V_x|$.

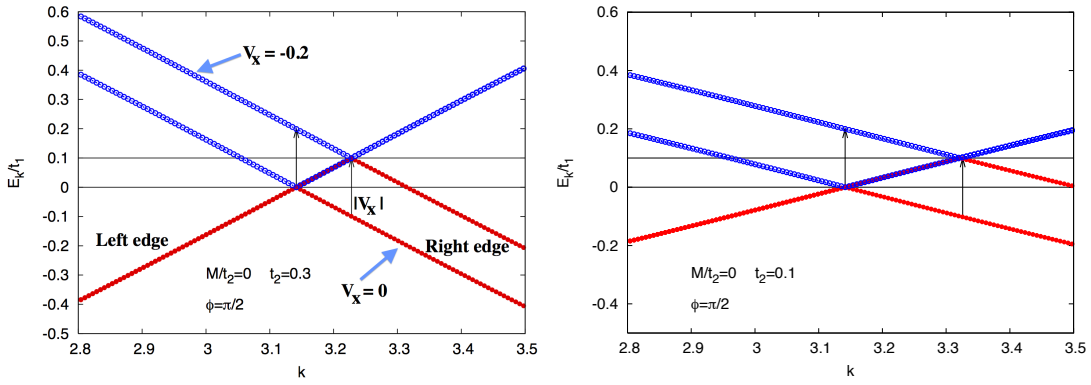

Figure 4.14.: (Left) A close-up view of the edge states, showing the effect of $V_x < 0$ on the right-edge states, which are shifted upwards by $|V_x|$. The new Fermi energy is indicated (upper horizontal line), showing an unbalance of occupied current-carrying states (filled red circles) when $V_x < 0$, which makes left edge states more populated. Here $t_2/t_1 = 0.3$. (Right) Same plot but for $t_2/t_1 = 0.1$, showing that the lower value of v_{k_y} is compensated by a higher density of states.

of all bands for $V_x/t_1 = -0.2$ (right) compared to the previously discussed results for $V_x = 0$ (left), both for $M = 0$ and $\phi = \pi/2$. The difference between the unperturbed values and those in presence of V_x is hardily noticeable on this scale. A closer look, however, reveals the differences induced by V_x: Fig. 4.13 compares the bulk and edge bands for $V_x/t_1 = -0.2$ with the unperturbed edge band at $V_x = 0$ (dashed line), zooming-in in a region close to the top of the valence band at $k_y = 0$ (left) or close to $k_y = 2\pi/a$ (right). We observe that the left edge is unaffected by the bias (recall that the extra potential felt by the electrons is essentially 0 close to the origin, where the left edge is located), while the right edge is almost perfectly shifted up in energy by $-V_x = |V_x|$ when $V_x < 0$. Due to this upward shift on the right edge band, the Fermi energy is also shifted up, by $|V_x|/2$, to keep the same half-filled situation as for $V_x = 0$, [26] as detailed in Fig. 4.14, from which it appears immediately that there is now an unbalanced situation of current-carrying states, with *more left edge states populated* when $V_x < 0$, as illustrated in the previous figures. This unbalance of currents at the two edges brings, for $V_x < 0$, an overall particle current going *upward*, i.e., an overall electrical current going *downward*.

The question is now why this unbalanced current is such that the Hall conductivity is exactly quantized in terms of e^2/h. One might be afraid of the fact that, after all, the slope of the edge states — hence the current v_{k_y} carried by each individual state of momentum k_y — is determined by parameters of the model, hence it is not universal. This is correct. Nevertheless, the change in v_{k_y}, as you change the parameters of the model, is compensated by a corresponding change in the *density of states* of such unbalanced edge states in the appropri-

[26] Notice that we have here a closed system with a conserved number of particles, in equilibrium. In reality, the voltage is applied through appropriate contacts and leads, which provide reservoirs of particles kept at different chemical potentials, $\mu_L - \mu_R = eV_x$. A correct description of this physics, of course, requires a non-equilibrium set-up.

ate energy window of width $|V_x|$, as illustrated by the right-panel of Fig. 4.14. This is exactly the type of argument used in deriving the Landauer formula for the ballistic current of a sub-band crossing the Fermi energy. Let us see how it works for the present context. By looking at Fig. 4.14 you realize that the k_y left-edge states which are not balanced by their partners at the right edge are exactly those whose energy falls within the region $[-e|V_x|/2, +e|V_x|/2]$ of the unperturbed Fermi energy $\varepsilon_F = 0$. Their net current $I_y = L_x \cdot J^e_y/(L_x L_y)$ is then:

$$I_y = -\frac{e}{L_y} \sum_{k_y}^{\text{window}} v_{k_y} \overset{L_y\to\infty}{=} -e \int_{\text{window}} \frac{dk_y}{2\pi}\, v_{k_y} \,, \tag{4.76}$$

But $v_{k_y} = \frac{1}{\hbar}\frac{\partial E_{\text{edge},-}(k_y)}{\partial k_y}$, and therefore: [27]

$$I_y = -e \int_{\text{window}} \frac{dk_y}{2\pi}\, \frac{1}{\hbar}\frac{\partial E_{\text{edge},-}}{\partial k_y} = -\frac{e}{2\pi\hbar}[E_{\text{up}} - E_{\text{low}}] = \frac{e^2}{h} V_x \,, \tag{4.77}$$

where we have used the fact that the energy window is $E_{\text{up}} - E_{\text{low}} = e|V_x| = -eV_x$. Hence:

$$I_y = \frac{e^2}{h} V_x \quad \Longrightarrow \quad \sigma_{yx} = \frac{I_y}{V_x} = \frac{e^2}{h} \,. \tag{4.78}$$

An opposite result, $\sigma_{yx} = -e^2/h$, is found in the other lobe of the topologically non-trivial Haldane phase diagram, because there the right-edge states have a *positive slope*.

4.7. Laughlin's argument

Soon after the experimental discovery by von Klitzing of the Integer Quantum Hall Effect (IQHE), in 1981, Laughlin wrote a remarkable two-page paper [19] explaining, through an argument relying on gauge invariance, why the Hall conductivity of an IQHE system should be quantized in multiples of e^2/h. The argument is deceptively simple, but hides many important facets — the role of disorder and the aspect of adiabaticity, for instance — which are not trivial at all. I would like to go through it in the present simple context, so that you get a concrete instance of its articulation.

The first idea of Laughlin was that of transforming the usual Hall-bar plane geometry into a cylinder — as we have done in the previous sections for the Haldane model on a strip — with the axis along the $\hat{\mathbf{x}}$-axis, and considering the effect of an inaccessible magnetic flux Φ_y piercing the cylinder along its axis. Laughlin stipulated that the IQH system was such that the Fermi energy was in the middle of a *mobility gap* — i.e., such that the longitudinal $\sigma_{xx} = 0$ — where the electronic states, albeit present, are localized in nature due to *disorder*, hence carry no current: so, disorder and localization of states in between otherwise sharp Landau level states are essential ingredients to the picture, and leads to something very similar to what we have in the insulating Haldane phase: a gap between current carrying

[27] Note that the density of states of the edge band is just the Jacobian in the change of variables from k to E:

$$\rho(E)dE = dk \qquad \Rightarrow \qquad \rho(E) = \frac{1}{\frac{dE}{dk}} = \frac{1}{\hbar v_k} \,.$$

states (the Landau levels), at least in the bulk. For a finite Hall-bar, like for the Haldane strip, the confining effect of the edges of the Hall-bar is such that *edge states* are generated out of the Landau levels: these edge states cross the bulk gap, pretty much as we have seen for the topological Haldane insulator. What Laughlin concluded was that, in such a case, by adiabatically increasing the inaccessibly flux Φ_y by one flux quantum $\phi_0 = hc/e$ one should provoke a transfer of an *integer multiple* of elementary charges e from one edge to the opposite one. Let us see why.

We follow here a route slightly different from the original paper by Laughlin, following rather Ref. [15, Sec. 4.7]. A (slow) linear increase of the inaccessible magnetic flux Φ_y along the cylinder axis generates, by Faraday's law $\boldsymbol{\nabla} \times \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}$ a constant-in-time electric field all around the cylinder axis, so that the cylinder strip surface will feel an electric field E_y. If you call C a contour of length L_y running along the circumference of the cylinder, and Σ the surface section enclosed by C and pierced in the center by Φ_y, then you immediately deduce, using Faraday's law, that:

$$L_y E_y = \oint_C \mathbf{E}_y \cdot d\mathbf{l} = \int_\Sigma (\boldsymbol{\nabla} \times \mathbf{E}) \cdot d\boldsymbol{\sigma} = -\frac{1}{c}\frac{d\Phi_y}{dt} \ . \tag{4.79}$$

This electric field E_y will in turn generate, in linear response theory, a current flowing in the x direction:

$$j_x^e = \sigma_{xy} E_y \quad \Rightarrow \quad \frac{dQ}{dt} = I_x = L_y j_x^e = \sigma_{xy} L_y E_y = -\sigma_{xy}\frac{1}{c}\frac{d\Phi_y}{dt} \ , \tag{4.80}$$

where we have also used that a current flowing in the $\hat{\mathbf{x}}$-direction implies a change of the charge Q at the edge according to $I_x = \frac{dQ}{dt}$. Integrating over time both sides, assuming the flux change in flux $\Delta\Phi_y$ is precisely a flux quantum ϕ_0 (recall that $\sigma_{xy} = -\sigma_{yx}$) we finally get:

$$\Delta Q = -\sigma_{xy}\frac{1}{c}\Delta\Phi_y = -\sigma_{xy}\frac{\phi_0}{c} = \sigma_{yx}\frac{h}{e} \ . \tag{4.81}$$

How much is ΔQ is the crucial issue. And here comes a further crucial observation: the insertion of a full flux quantum ϕ_0 leads to a final Hamiltonian $\widehat{H}(\Phi_y = \phi_0)$ which is *unitarily equivalent* to the initial Hamiltonian without flux

$$\widehat{H}(\Phi_y = \phi_0) \equiv \widehat{H}(\Phi_y = 0) \ , \tag{4.82}$$

hence the spectrum of both Hamiltonians is the same. Nevertheless, the time-dependent Schrödinger dynamics with an adiabatic ramp-up of the flux Φ_y, starting from the ground state of $\widehat{H}(0)$ *does not necessarily* lead back to the ground state, but rather to an exited state, which can be argued to correspond to a transfer of an *integer number* n of electrons from one edge to the other:

$$\Delta Q = ne \quad \Rightarrow \quad \sigma_{yx} = \frac{ne^2}{h} \ , \tag{4.83}$$

the integer n depending on the number of edge modes crossing the bulk gap. Let us examine better the reason why $\Delta Q = ne$, with the example of our Haldane strip edge states.

Let us consider, for definiteness, the highly symmetric topological insulator point with $M = 0$ and $\phi = \pi/2$, whose edge states are shown in Fig. 4.9. Fig. 4.15 shows a zoom

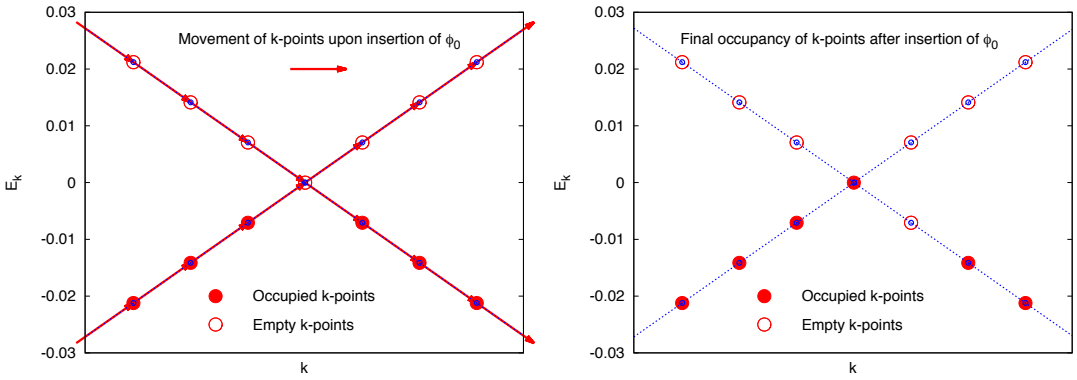

Figure 4.15.: A zoom on the edge states close to the crossing point at $k_c = \pi/a$. For simplicity of argumentation, the quasi-degenerate states at k_c are considered to be initially empty.

of the two edge bands close to the crossing point at $k_c = \pi/a$, where the discrete k-points due to a finite L_y are visible. You notice that the point at k_c appears as a true crossing of the bands, but is in reality — as previously discussed — an *avoided crossing* although with a exponentially small gap $\mathrm{e}^{-\alpha L_x}$ that is very difficult to see numerically for small L_x, and absolutely beyond numerical grasp for physically sensible values of L_x. [28] Assume that we start, see left panel of Fig. 4.15 with a Slater determinant where the k_y points denoted by filled red circles are occupied, while the others are empty. For simplicity of argumentation, assume that the filling is slightly defective so that the quasi-degenerate k_c point is initially empty. Now we slowly ramp-up the flux $\Phi_y(t)$ as a function of time as $\Phi_y = \lambda t$, corresponding by Faraday's law to putting a small electric field in the $\hat{\mathbf{y}}$-direction and making the κ_y time-dependent:

$$E_y = -\frac{1}{cL_y}\frac{d\Phi_y}{dt} = -\frac{\lambda}{cL_y} \quad \text{and} \quad \kappa_y(t) = \frac{2\pi}{L_y}\frac{\lambda t}{\phi_0} \,. \tag{4.84}$$

If λ is sufficiently small — but not *infinitely* small, see below —, the adiabatic theorem will be respected almost everywhere, and the time-evolved state is essentially the Slater determinant made-up of the same filled k_y-points, but at shifted momenta $k_y + \kappa_y(t)$. But there is a point where adiabaticity cannot be maintained: this is the avoided-crossing point, where we are actually in presence of a *Landau-Zener* type of problem with an exponentially small gap $\mathrm{e}^{-\alpha L_x}$, and the system will not be able to actually "follow the ground state". After a time T such that $\Phi_y(T) = \lambda T = \phi_0$, we have that $\kappa_y(T) = \frac{2\pi}{L_y}$, i.e., each $k_y = \frac{2\pi}{L_y}n$ has now been shifted to $k_y + \kappa_y(T) = \frac{2\pi}{L_y}(n+1)$: the whole set of k_y-points is therefore indistinguishable from those without Φ_y, but the occupation of the k_y-points is different from the initial one! Indeed, the occupied left-edge mode at $k_c - \frac{2\pi}{L_y}$ is brought (still occupied) into a left-edge mode at k_c (which is not an eigenstate at k_c), while the initially empty mode at k_c is now seen as an empty right-edge mode at $k_c + \frac{2\pi}{L_y}$, which was formerly occupied. The shift of k_y points towards the right — in a kind of chain reaction, like when someone pushes inside

[28] For the case illustrated in the figures, where $L_x = 64a$, such a gap is still numerically visible, $\hbar\Delta \approx 4\times10^{-10}$. But any reasonable mesoscopic value of L_x would bring an ultra-tiny value of $\hbar\Delta$ which makes adiabaticity violated during the flux insertion, for all practical insertion rates.

a queue and the whole queue advances by one unit — involves evidently a transfer of one electron from the right-edge towards the left edge. Such a transfer, however, does not occurr through an unphysical direct tunneling from right to left, but rather via a whole chain of edge and bulk states — the latter being those at the top of the valence band — involved in the shift. The following animation illustrates this transfer.

To end this section, I should stress that the original argument was actually formulated in a way that is slightly different from that given above. To show quantization, Laughlin actually starts from Eq. (4.62) and argues that:

$$I_y = -c\frac{\partial E_0(\Phi_y)}{\partial \Phi_y} \Rightarrow I_y = -c\frac{\Delta U}{\Delta \Phi_y} \,, \tag{4.85}$$

where ΔU is the adiabatic change in total energy during the slow insertion of the flux $\Delta\Phi_y = \phi_0$. Now, when a charge $\Delta Q = ne$ is transported across the bulk sample from one edge to the other, there is an adiabatic total energy change $\Delta U = -neV_x$, where V_x is the voltage bias across the strip/bar. Hence, again, you find:

$$I_y = c\frac{neV_x}{\phi_0} = \frac{ne^2}{h}V_x \,. \tag{4.86}$$

The difficulty with showing that there is actually a finite total energy change in our calculation on the Haldane strip is that we do not do the actual physical calculation, which would require an open system with two leads attached at different chemical potentials acting as particle reservoirs. As a consequence of that, in our "canonical calculation" it rather seems that the particle-hole excitation created by the adiabatic insertion of flux has always a *small* excitation energy, of the order of $\sim \Delta k_y = 2\pi/L_y$. This is the reason why we rephrased the argument in terms of the adiabatically transported charge ΔQ, rather then in terms of the adiabatic energy change ΔU. But the essence of the argument is identical, I believe. One slight advantage of the formulation in terms of ΔQ is that it immediately shows that you do not need a finite V_x to show that there is a quantized conductance. As obvious from the linear response theory framework, the quantized conductance is a property of the unperturbed system at $V_x = 0$, and the fact that the adiabatically transported charge is $\Delta Q = ne$ even when $V_x = 0$ shows the result in a particularly transparent way.

4.8. Thouless adiabatic charge pump

The Laughlin's argument presented in the previous section hinges on the crucial point that the charge transferred between the two edges of an IQH system during the adiabatic insertion of a full quantum ϕ_0 of inaccessible flux must be quantized: $\Delta Q = ne$. Soon after, Thouless wrote a beautiful paper [8] in which he explained why the electronic charge adiabatically transported in infinite lattice-periodic insulators must always be quantized. This very nice paper might be the subject for an end-of-course seminar. If you are interested, see the original paper [8], and R. Resta's lecture notes [4, Sec. 4.6 and Chap. 5], where the connection to the modern theory of electronic polarization is explained in detail.

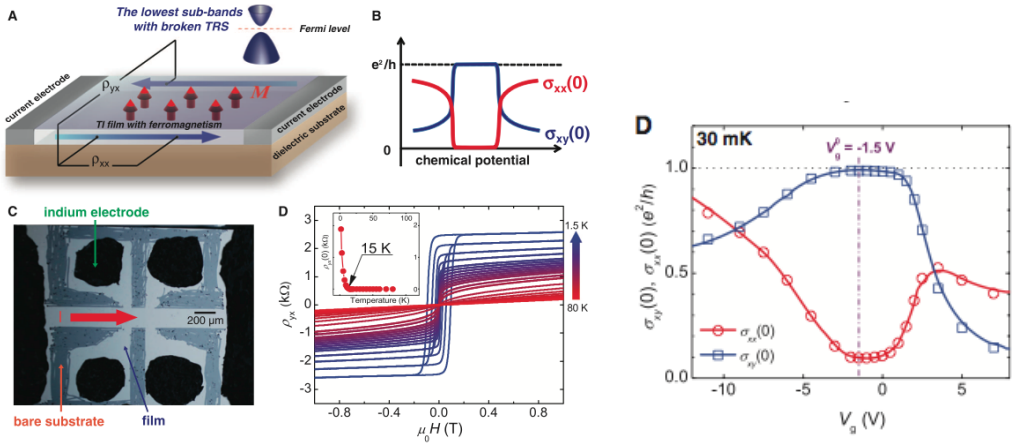

Figure 4.16.: Figure taken from the original reference of C.Z. Chang *al.*, Science **340**, 167 (2013), showing the experimental realization of Haldane's idea.

4.9. The effect of disorder

Any realistic system has disorder in it. It is therefore important to ask how robust are the effects we have just described against disorder. In the present context the crucial idea is that disorder can lead to back-scattering of states only when states of opposite momentum are available. Here the left edge states are all chiral and transport current only in one direction. A back-scattering mechanism therefore, would need to involve a transition to states with opposite chirality/momentum, which however live on the other edge! Therefore, the usual back-scattering mechanism is ineffective in a situation with edge states like in the Haldane problem, and you expect the system to be rather robust against disorder. If you are interested, you can look at the literature on Topological Anderson Insulators, for instance [20, 21].

4.10. The experimental realization

Good ideas can stay quiescent for decades, but in the end they reemerge. Haldane's paper was basically not cited for almost 30 years, until Kane and Mele realized how profound it was. But even more surprising is perhaps the fact that an experimental realization of Haldane's idea, almost literal, has been recently performed. The experiment is described in Ref. [13]: it is known as Quantum Anomalous Hall Effect (QAHE). I will not enter into a detailed discussion of the experiment. The interested reader can consult the original paper.

5. The Quantum Spin Hall Effect

5.1. The Kane-Mele model

In 2005 Kane and Mele [14, 22] introduced a model for graphene that is deeply based on the Haldane model [12] we have just discussed. One crucial difference is that Kane and Mele explicitly consider the role of the electron *spin*, and write down a *spin-orbit* coupling term in a way that ends up being essentially identical to the t_2 next-nearest-neighbor (nnn) hopping introduced by Haldane, except that electrons with spin $\uparrow$ (we label them with $s = +$) have a Haldane flux $\phi = \frac{\pi}{2}$, while electrons with spin $\downarrow$ (here $s = -$) have a flux $\phi = -\frac{\pi}{2}$. On top of that, Kane and Mele discuss the role of other spin-orbit-related terms which induce spin-flip terms. The Kane-Mele model, with our old notation, might be written as: [1]

$$\begin{aligned}\hat{H}_{\rm KM} &= t_1 \sum_{s=\pm}\sum_{\mathbf{r}\in A}\sum_{\mathbf{d}_j}\left(\hat{c}^\dagger_{\mathbf{r}+\mathbf{d}_j s}\hat{c}_{\mathbf{r}s} + \text{H.c.}\right) + \underbrace{t_2 \sum_{s=\pm}\sum_{\mathbf{r}}\sum_{\mathbf{a}_j}\left(is\nu_{\mathbf{r}\to\mathbf{r}+\mathbf{a}_j}\hat{c}^\dagger_{\mathbf{r}+\mathbf{a}_j s}\hat{c}_{\mathbf{r}s} + \text{H.c.}\right)}_{\hat{H}_{\rm SO}} \\ &\quad + \sum_{s=\pm}\sum_{\mathbf{r}} M_{\mathbf{r}}\hat{c}^\dagger_{\mathbf{r}s}\hat{c}_{\mathbf{r}s} + \text{ Spin-flip terms} \\ &= \sum_{s=\pm}\hat{H}^{(s)}_{\rm Hal}(\phi = s\tfrac{\pi}{2}) + \text{ Spin-flip terms}\,. \end{aligned} \tag{5.1}$$

Notice that the $is\nu_{\mathbf{r}\to\mathbf{r}+\mathbf{a}_j} = \pm i$ is exactly what you get from the Haldane model phase factor $e^{i\phi\nu_{\mathbf{r}\to\mathbf{r}+\mathbf{a}_j}}$ for $\phi = s\frac{\pi}{2}$. Here $\hat{H}^{(s)}_{\rm Hal}(\phi)$ denotes a Haldane-model with Haldane-flux ϕ for the electrons with spin $s = \pm$. We want to stress that, at variance with the Haldane model, there is really no external magnetic field here. The system is perfectly *time-reversal invariant* (see later for more comment on this crucial issue), and the whole job is done by the *spin-orbit coupling* term, which we can microscopically write as: [2]

$$\hat{V}_{\rm SO} = \frac{e\hbar}{2m^2c^2}\hat{\mathbf{S}}\cdot(\mathbf{E}\times\hat{\mathbf{p}}) = \frac{\hbar}{2m^2c^2}\hat{\mathbf{S}}\cdot(\boldsymbol{\nabla}V\times\hat{\mathbf{p}})\,, \tag{5.2}$$

where $V(\mathbf{x})$ is the crystalline potential that the electrons in graphene feel.

How is it, you might ask, that spin-orbit leads to such a Haldane-like nnn-hopping term? A microscopic derivation, briefly mentioned by Kane and Mele [14, p. 4], is a bit cumbersome, although not difficult. I give a somewhat detailed account of the main steps behind this derivation in Appendix B. Symmetry, of course, is a very good tool to get the result, at least

[1] The notation of Kane and Mele [14, Eq. 6] is slighly different. They use $\langle\langle ij\rangle\rangle$ to indicate nnn hopping on the same sublattice, and $\nu_{ij} = \pm 1$ on sublattice A or B, respectively. Moreover, they indicate $t_2 \leftrightarrow \lambda_{SO}$ and $M \leftrightarrow \lambda_v$.

[2] We use here that $\mathbf{E} = -\boldsymbol{\nabla}\Phi_e$, hence $e\mathbf{E} = \boldsymbol{\nabla}V$ where $V = -e\Phi_e$. Moreover, the spin operator $\hat{\mathbf{S}}$ is assumed to be dimensionless.

in a continuum Dirac description of the underlying physics [14, 22]. There are a few things that are not difficult to grasp, however. The relevant orbitals that form the two Dirac-cone bands of graphene are the $2p_z$-like $\phi_\pi(\mathbf{x})$ orbitals centered at the Carbon sites: if x, y denote the coordinates on the graphene plane, and z the coordinate orthogonal to the plane, the ϕ_π orbitals have a definite parity, *odd*, under $z \to -z$. The same parity under $z \to -z$ is inherited, as a consequence, by the Bloch states $\psi_{\mathbf{k}n}(\mathbf{x})$ of the two Dirac bands. Therefore, if we consider for instance the spin-orbit contribution

$$\hat{S}_x(\boldsymbol{\nabla} V \times \hat{\mathbf{p}})_x = \hat{S}_x\Big((\partial_y V)\,\hat{p}_z - (\partial_z V)\,\hat{p}_y\Big)$$

we realize that it *must have vanishing* matrix elements between the relevant Bloch band states, because both $\partial_z V$ and $\hat{p}_z$ are *odd* under $z \to -z$. A similar argument applies to $\hat{S}_y(\boldsymbol{\nabla} V \times \hat{\mathbf{p}})_y$. Therefore, in the low-energy sector involving the two Dirac-bands, the only relevant (surviving in lowest-order perturbation theory) spin-orbit term is the $\hat{S}_z$-one:

$$\hat{V}_{\rm SO} \overset{low-energy}{\Longrightarrow} \frac{\hbar}{2m^2c^2}\,\hat{S}_z\,\Big((\partial_x V)\,\hat{p}_y - (\partial_y V)\,\hat{p}_x\Big)\,, \tag{5.3}$$

This fact implies that, to lowest order in perturbation theory, we need not worry about *spin-flip* processes: the spin operator $\hat{S}_z$ is (approximately) conserved. Moreover, we immediately see that the *sign* of the term is *opposite* for electrons with spin $\uparrow$ and electrons with spin $\downarrow$. A rough estimate for such spin-orbit coupling proves it quite small, compared to the nearest-neighbor overlap $t_1 \approx -2.8$ eV:

$$t_2 = \lambda_{\rm SO} \sim \frac{\hbar}{4m^2c^2}\langle(\partial_x V)\,\hat{p}_y\rangle \sim \frac{\hbar}{4m^2c^2}\frac{e^2}{a^2}\frac{2\pi\hbar}{3a} \sim \frac{\pi\hbar^2e^2}{6m^2c^2a^3} \sim 0.1\ \text{K} \sim 9\ \mu\text{eV}\,. \tag{5.4}$$

To fully justify the tight-binding form given above, it would remain to show that: *1)* there are no spin-orbit matrix elements betweeen states living on opposite sublattices, i.e., only AA- or BB-terms are really possible, and *2)* that the relevant matrix elements for Bloch states exactly at the Dirac cones have *opposite sign* for the two sublattices (indeed, in a real space tight-binding description you have $+it_2$ on sublattice A and $-it_2$ on sublattice B). A proof of the fact that there are no other phase factors, except for a minus sign change between A and B, requires a more detailed analysis: Appendix B contains most of the details. I give a short account of the story in the next subsection.

I should mention, however, that Kane and Mele consider also another spin-orbit contribution, the so-called *Rashba term*, which arises when there is an external electric field $\mathbf{E} = E_z\hat{\mathbf{z}}$ acting along the z-direction – be it due to an actual electric field, or simply to an asymmetry of the crystalline potential due to a *substrate* on which the graphene is laid. Such a term would have the miscroscopic form:

$$\hat{V}_{\rm R} = \frac{e\hbar}{2m^2c^2}\hat{\mathbf{S}}\cdot(\mathbf{E}\times\hat{\mathbf{p}}) = \frac{e\hbar}{2m^2c^2}E_z\,\hat{\mathbf{z}}\cdot(\hat{\mathbf{p}}\times\hat{\mathbf{S}}) = \frac{e\hbar}{2m^2c^2}E_z\,(\hat{p}_x\hat{S}_y - \hat{p}_y\hat{S}_x)\,. \tag{5.5}$$

The Rashba term involves, as it is clear from the presence of $\hat{S}_{x,y}$, *spin-flips* of the Dirac electrons: the Hamiltonian can no-longer be written as the direct sum of one for spin $s = +$ and one for $s = -$, i.e., *spin-flip* processes are necessarily present, and the analysis is considerably more complicated. These terms, and others originating in higher-order in perturbation theory, make $\hat{S}_z$ only an *approximately* conserved quantity. We can estimate the coupling

constant λ_R of the Rashba term by realizing that $\langle \hat{p}_{x,y} \rangle \sim m v_F$, where v_F is the Fermi velocity of the Dirac-cone dispersion, hence: [14]

$$\lambda_{\rm R} \sim \frac{\hbar v_F e E_z}{4mc^2} \sim 0.5 \text{ mK} \sim 0.04 \ \mu\text{eV} \ , \tag{5.6}$$

where we have assumed that the electric field is $E_z = 50\,\text{V}/(300\,\text{nm})$.

5.1.1. The ordinary spin-orbit term as an Haldane t_2 term.

Let us denote by $\phi_\pi(\mathbf{x}-\mathbf{r}) = \langle \mathbf{x}|\hat{c}^\dagger_{\mathbf{r}}|0\rangle$, or even more compactly as $\phi_{\mathbf{r}}(\mathbf{x})$, the $2p_z$-like π-orbital [3] centered on the Carbon atom sitting at the lattice position $\mathbf{r}$. We can form Bloch sums restricted on the two sublattices $a = A, B$ as follows:

$$\begin{aligned} \psi_{a\mathbf{K}_\pm}(\mathbf{x}) &= \langle \mathbf{x}| \frac{e^{i\theta_{a\mathbf{K}_\pm}}}{\sqrt{N}} \sum_{\mathbf{r}_a} e^{i\mathbf{K}_\pm\cdot\mathbf{r}_a} \hat{c}^\dagger_{\mathbf{r}_a}|0\rangle = \frac{e^{i\theta_{a\mathbf{K}_\pm}}}{\sqrt{N}} \sum_{\mathbf{r}_a} e^{i\mathbf{K}_\pm\cdot\mathbf{r}_a} \phi_\pi(\mathbf{x}-\mathbf{r}_a) \\ &= e^{i\mathbf{K}_\pm\cdot\mathbf{x}} \underbrace{\frac{e^{i\theta_{a\mathbf{K}_\pm}}}{\sqrt{N}} \sum_{\mathbf{r}_a} e^{i\mathbf{K}_\pm\cdot(\mathbf{r}_a-\mathbf{x})} \phi_\pi(\mathbf{x}-\mathbf{r}_a)}_{u_{a\mathbf{K}_\pm}(\mathbf{x}) \text{ periodic}} = e^{i\mathbf{K}_\pm\cdot\mathbf{x}}\, u_{a\mathbf{K}_\pm}(\mathbf{x}) \ . \end{aligned} \tag{5.7}$$

Here $\mathbf{r}_{a=A(B)}$ denote the $\mathbf{r}$-sites on the $A(B)$ sublattice, respectively. Notice that we have introduced an overall phase $\theta_{a\mathbf{K}_\pm}$ whose usefulness is appreciated in deriving the Dirac equation. The final step shows how to extract the periodic part $u_{a\mathbf{K}_\pm}(\mathbf{x})$. [4] By diagonalizing the 2×2 tight-binding problem on this basis of Bloch-states, we can easily express the actual tight-binding Bloch eigenstates $\psi_{\mathbf{K}_\pm, n=1,2}$ in terms of $\psi_{A\mathbf{K}_\pm}$ and $\psi_{B\mathbf{K}_\pm}$. Let us now introduce a combined index $\mathrm{a} = a\mathbf{K}_\alpha$, running over the *four* values

$$\mathrm{a} \to (A\mathbf{K}_+, B\mathbf{K}_+, A\mathbf{K}_-, B\mathbf{K}_-)$$

to have shorthand notation, so that $\psi_{a\mathbf{K}_\pm}(\mathbf{x}) \to \psi_{\mathrm{a}}(\mathbf{x})$. As previously discussed, we can effectively keep only the $\hat{S}_z$ spin-orbit term at low energies. Within first-order degenerate perturbation theory, we would need to calculate the following 4×4 matrix:

$$\langle \psi_{\mathrm{a}} | (\boldsymbol{\nabla} V \times \hat{\mathbf{p}})_z | \psi_{\mathrm{a}'} \rangle \ . \tag{5.8}$$

Let us look first at the basic matrix elements of the $\phi_{\mathbf{r}_a}(\mathbf{x})$ orbitals centered on the Carbon atoms. We notice that:

$$\langle \phi_{\mathbf{r}_A+\mathbf{d}_3} | \Big[(\partial_x V)\, \hat{p}_y - (\partial_y V)\, \hat{p}_x \Big] | \phi_{\mathbf{r}_A} \rangle = 0 \ , \tag{5.9}$$

because both terms are *odd* under $y \to -y$ aroud the $\mathbf{r}_A \to \mathbf{r}_A + \mathbf{d}_3$ bond, which is along the x axis (the first because of $\hat{p}_y$, the second because of $\partial_y V$). Rotational symmetry by $\pm 2\pi/3$ around the z-axis immediately implies that quite generally:

$$\langle \phi_{\mathbf{r}_A+\mathbf{d}_j} | (\boldsymbol{\nabla} V \times \hat{\mathbf{p}})_z | \phi_{\mathbf{r}_A} \rangle = 0 \quad \Rightarrow \quad \langle \psi_{B\mathbf{K}_\pm} | (\boldsymbol{\nabla} V \times \hat{\mathbf{p}})_z | \psi_{A\mathbf{K}_\pm} \rangle = 0 \ . \tag{5.10}$$

[3] Appropriately orthonormalized to the neighboring ones by the Löwdin method, or simply neglecting the small overlaps between orbitals on different sites.

[4] The proof that $u_{a\mathbf{K}_\pm}(\mathbf{x})$ are lattice-periodic is elementary.

Similar conclusions apply to the inter-valley (i.e., coupling different Dirac cones) elements $\langle\psi_{B\mathbf{K}_\mp}|(\boldsymbol{\nabla}V\times\hat{\mathbf{p}})_z|\psi_{A\mathbf{K}_\pm}\rangle = 0$.

Next we consider the other relevant matrix element: $\langle\phi_{\mathbf{r}_A+\mathbf{a}_3}|(\boldsymbol{\nabla}V\times\hat{\mathbf{p}})_z|\phi_{\mathbf{r}_A}\rangle$. Here we notice that:

$$\langle\phi_{\mathbf{r}_A+\mathbf{a}_3}|\Big[(\partial_x V)\,\hat{p}_y - (\partial_y V)\,\hat{p}_x\Big]|\phi_{\mathbf{r}_A}\rangle = -i\hbar C \neq 0\,, \tag{5.11}$$

because both $\partial_x V$ and $\partial_y V$ have *no definite parity* under $x\to -x$ around the bond $\mathbf{r}_A \to \mathbf{r}_A+\mathbf{a}_3$. Moreover, a careful look at the lattice structure shows that the *sign* of $\partial_x V$ and $\partial_y V$ is exactly opposite in the corresponding integral for the B-sublattice, i.e.,

$$\langle\phi_{\mathbf{r}_B+\mathbf{a}_3}|\Big[(\partial_x V)\,\hat{p}_y - (\partial_y V)\,\hat{p}_x\Big]|\phi_{\mathbf{r}_B}\rangle = +i\hbar C \neq 0\,. \tag{5.12}$$

These results, obtained for the $\mathbf{a}_3$-bond, extend by $\pm 2\pi/3$ rotational symmetry around the z-axis to all the $\mathbf{a}_j$ bonds. Summarizing, we have:

$$\langle\phi_{\mathbf{r}_B+\mathbf{a}_j}|(\boldsymbol{\nabla}V\times\hat{\mathbf{p}})_z|\phi_{\mathbf{r}_B}\rangle = -\langle\phi_{\mathbf{r}_A+\mathbf{a}_j}|(\boldsymbol{\nabla}V\times\hat{\mathbf{p}})_z|\phi_{\mathbf{r}_A}\rangle = +i\hbar C \neq 0\,. \tag{5.13}$$

At this point it is straightforward to evaluate:

$$\begin{aligned}\langle\psi_{A\mathbf{K}_\pm}|(\boldsymbol{\nabla}V\times\hat{\mathbf{p}})_z|\psi_{A\mathbf{K}_\pm}\rangle &= \frac{1}{N}\sum_{\mathbf{r}_A}\Big(\sum_{\mathbf{a}_j} e^{-i\mathbf{K}_\pm\cdot\mathbf{a}_j}\langle\phi_{\mathbf{r}_A+\mathbf{a}_j}|(\boldsymbol{\nabla}V\times\hat{\mathbf{p}})_z|\phi_{\mathbf{r}_A}\rangle + c.c.\Big)\\ &= \sum_{\mathbf{a}_j}\Big(-i\hbar C e^{-i\mathbf{K}_\pm\cdot\mathbf{a}_j} + c.c.\Big) = \pm 3\sqrt{3}\hbar C\,.\end{aligned} \tag{5.14}$$

Adding the spin-orbit term exactly at the BZ corners (i.e., at $\mathbf{q}=0$) as a perturbation to the Dirac term (see Appendix B) we would write the effective mass Hamiltonian in momentum space as:

$$\left[\begin{array}{cc|cc} s\Delta_{\rm SO} & \hbar v_F(q_x+iq_y) & 0 & 0\\ \hbar v_F(q_x-iq_y) & -s\Delta_{\rm SO} & 0 & 0\\ \hline 0 & 0 & -s\Delta_{\rm SO} & \hbar v_F(q_x-iq_y)\\ 0 & 0 & \hbar v_F(q_x+iq_y) & s\Delta_{\rm SO}\end{array}\right] \tag{5.15}$$

where $s=+$ for the $\uparrow$-electrons, and $s=-$ for $\downarrow$ ones, while $\Delta_{\rm SO}$, collecting all factors, is:

$$\Delta_{\rm SO} = \frac{\hbar}{2m^2c^2}\frac{3\sqrt{3}}{2}\hbar C\,. \tag{5.16}$$

In a more compact form, we write this as:

$$\mathcal{H}(\mathbf{q}) = \mathcal{H}_0(\mathbf{q}) + \mathcal{H}_{\rm SO} = \hbar v_F\,[q_x\hat{\sigma}_x - q_y\hat{\tau}_z\hat{\sigma}_y] + \Delta_{\rm SO}\hat{s}_z\hat{\tau}_z\hat{\sigma}_z\,. \tag{5.17}$$

5.2. The Quantum Spin Hall Effect

It is simple to show that there is a spin conductivity in the Kane-Mele model, but its value is only *approximately* quantized, due to the presence of the previously mentioned spin-flip terms. As such, the spin-conductivity itself can hardly be considered as a topological quantity.

Consider the up-spin number current $I_y^{\uparrow}$, i.e., the current omitting the charge factor $-e$. If we omit altogether the spin-flip terms, the model is a sum of two independent Haldane models with opposite fluxes for the two spin species. Therefore we have:

$$I_y^{\uparrow} = -\frac{e}{h} V_x \ , \tag{5.18}$$

due to an unbalance between the left-edge modes, and the right-edge ones, as previously discussed. A similar unbalance occurs for the down-spin number current $I_y^{\downarrow}$, which has however opposite sign:

$$I_y^{\downarrow} = +\frac{e}{h} V_x \ . \tag{5.19}$$

The two currents cancel, if you look at the total charge current $I_y^e = (-e)(I_y^{\uparrow} + I_y^{\downarrow}) = 0$. But if you define the spin current $I_y^{\rm spin} = \frac{\hbar}{2}(I_y^{\uparrow} - I_y^{\downarrow})$, the result is non-vanishing, and given by:

$$I_y^{\rm spin} = \frac{\hbar}{2}\left(-2\frac{e}{h}V_x\right) = -\frac{e}{2\pi}V_x = \sigma_{yx}^{\rm spin} V_x \ , \tag{5.20}$$

i.e., the spin-conductivity is

$$\sigma_{yx}^{\rm spin} = -\frac{e}{2\pi} \ . \tag{5.21}$$

It is important to stress that the spin-current is quantized in terms of the $\sigma_{yx}^{\rm spin}$ given above only insofar we neglect the spin-flip terms due to the Rashba spin-orbit coupling, and higher order spin-orbit induced spin-flip terms.

The only clear symmetry that a Hamiltonian surely has, in presence of spin-orbit, is *time-reversal* (TR): recall that both $\hat{\mathbf{p}}$ and $\hat{\mathbf{S}}$ are odd under TR, but $\hat{\mathbf{S}}\cdot(\mathbf{E}\times\hat{\mathbf{p}})$ is TR-invariant. Recall the expression for the Hall conductivity of a two-dimensional band insulator in Eq. (4.51):

$$\sigma_{yx} = \frac{e^2}{h}\frac{1}{2\pi}\sum_n^{\rm filled}\int_{\rm BZ} {\rm d}^2\mathbf{k}\; i\Big[\langle\partial_{k_x}u_{n\mathbf{k}}|\partial_{k_y}u_{n\mathbf{k}}\rangle - \langle\partial_{k_y}u_{n\mathbf{k}}|\partial_{k_x}u_{n\mathbf{k}}\rangle\Big] \ . \tag{5.22}$$

You can prove that, if TR is respected, the integrand appearing in σ_{yx} is an *odd* function of $\mathbf{k}$ [4, Sec. 3.7]; that implies, quite generally, that you do not expect any transverse charge conductivity σ_{yx}, *alias* TR-invariant systems are trivial Chern insulators.

Nevertheless, if you study the problem on a strip, you notice that there are edge states crossing the gap, and these survive even in presence of spin-flip terms: therefore, although the spin-conductivity is not topological, there must be *something* that distinguishes insulators of the trivial type from those that show non-trivial edge states. Fig. 5.1 shows the edge states obtained in the simple $\hat{S}_z$-conserving case; they are obtained by taking the edge states of two Haldane's model with $\phi = \pm\pi/2$ for the two opposite spin species. Observe in particular the exact crossing of the two opposite spin-edge states, living on the same physical edge, which occurs at $k = \pi/a$: these are Kramers degenerate pairs, as we shall discuss in the next Section, and you can argue that they must be there even in presence of Rashba or other spin-orbit spin-flipping terms. Indeed, the band structure so obtained is very similar to that presented by Kane and Mele [22, Fig.1] in presence of λ_R, which is reported in Fig. 5.2.

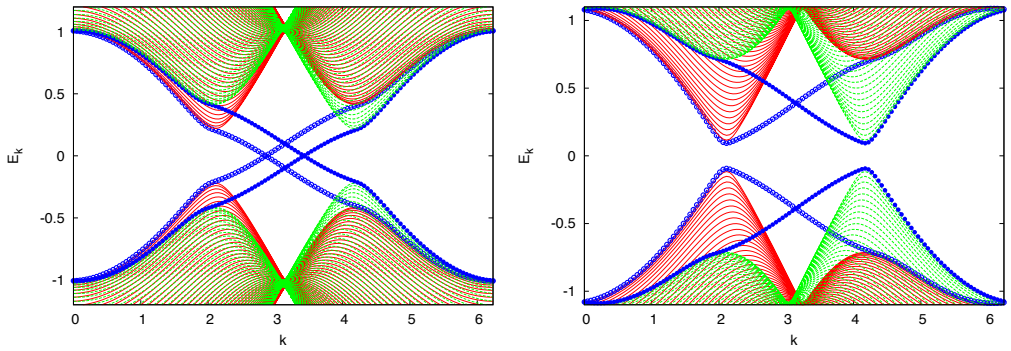

Figure 5.1.: Edge states for the Kane-Mele model in absence of Rashba coupling, $\lambda_R = 0$, for two values of the mass parameter $M = \lambda_v$: $\lambda_v = 0.1t_1$ (left), and $\lambda_v = 0.4t_1$ (right). In both cases $t_2 = 0.06t_1$. The open symbols and red curves refer to $\uparrow$ spin states, the closed symbols and green curves to $\downarrow$ spin curves. Notice that the edge states of opposite spin, but living on the same edge, exactly cross at $k_y = \pi/a$, as demanded by Kramers' theorem. The structure of the bands would be very similar in presence of a sufficiently small λ_R, with the same Kramer's degeneracy of more complicated spin-orbitals edge states.

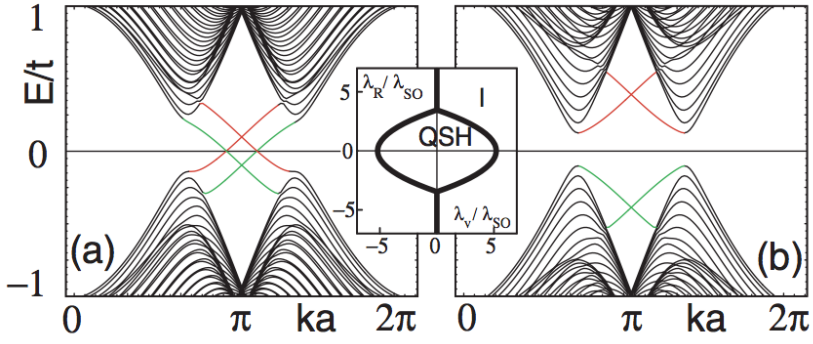

Figure 5.2.: Same as previous figure, with the same parameters, but in presence of a Rashba term $\lambda_R = 0.05t_1$. Figure taken from the original paper [22].

5.3. The importance of Time-Reversal

Time reversal symmetry is introduced in some detail in Appendix C. It is clear that the presence of spin-orbit mantains TR symmetry of the full Hamiltonian, $\hat{T}_R \hat{H} \hat{T}_R^{-1} = \hat{H}$. Since we are dealing with spin-1/2 systems, we know that $\hat{T}_R^2 = -\mathbb{1}$, and this in turn implies that every eigenstate must be *doubly degenerate* (Kramers theorem).

Suppose now that $\hat{H}$ has translational symmetry, such that you can write $\hat{H} = \sum_{\mathbf{k}}^{\mathrm{BZ}} \hat{H}(\mathbf{k})$. Then, since the momentum is odd under TR, you can show that:

$$\hat{T}_R \hat{H}(\mathbf{k}) \hat{T}_R^{-1} = \hat{H}(-\mathbf{k}) \; . \tag{5.23}$$

For generic values of $\mathbf{k}$, Kramers degeneracy is realized by the fact that each band n has a "inversion-reflected" partner band n' such that $\epsilon_{n'}(-\mathbf{k}) = \epsilon_n(\mathbf{k})$. When spin-orbit is not present, one can have extra degeneracies for the *same* value of $\mathbf{k}$, for instance $\epsilon_{n\uparrow}(\mathbf{k}) = \epsilon_{n\downarrow}(\mathbf{k})$), in general, any spin-orbit coupling would remove such degenerarices.

The relationship (5.23) immediately implies that there are $\mathbf{k}$-points that are left invariant by TR. Notably, the Γ-point $\mathbf{k} = 0$ is left invariant. But also the 3 points M in the middle of the faces of the standard Wigner-Seitz BZ — $M_1 = \mathbf{b}_1/2$, $M_2 = \mathbf{b}_2/2$, $M_3 = (\mathbf{b}_1 + \mathbf{b}_2)/2$ — are left invariant, because $-\mathbf{k}$ is equivalent to $\mathbf{k}$ via a reciprocal lattice vector $\mathbf{G}$:

$$-\mathbf{k} = \mathbf{k} + \mathbf{G} \qquad \longrightarrow \qquad 2\mathbf{k} = \mathbf{G} \; . \tag{5.24}$$

Such $\mathbf{k}$-points — often known as *time-reversal invariant momenta* (TRIM) — are rather special, because in essence you have that $\hat{T}_R \hat{H}(\mathbf{k}) \hat{T}_R^{-1} = \hat{H}(-\mathbf{k}) = \hat{H}(\mathbf{k})$, hence their $\mathbf{k}$-Hamiltonian is TR-invariant. Hence, Kramers degeneracy must occur *within* the same $\mathbf{k}$-subspace.

Let us picture now how edge states occurring in the middle of a bulk gap for a TR-invariant system might look like. Fig. 5.3(a) shows a sketch of 4 edge state bands in the bulk gap, two of them totally within the gap, two other only partially so. The solid circles correspond to TRIM, here $k_y = 0$ and $k_y = +\pi/a \equiv -\pi/a$. Each band has a time-reversal partner that we have denoted with different colors: a blue band is the Kramers degeneracy partner of a red band. Notice how red and blue bands (Kramers partners) join at the TRIM points, where the degeneracy occurs "at the same $\mathbf{k}$ point". Although we have plotted edge states here, the situation depicted is rather that of a *trivial insulator*. Indeed, depending on the number of electrons in the system, and on the detailed shape of the bands, the Fermi energy might cut the bands in 2 points in the interval $[0, \pi/a]$ (and other 2 points in the interval $(-\pi/a, 0]$), or in 0 points. Consider now Fig. 5.3(b), showing a similar sketch of edge states in the bulk gap: notice that the energy eigenvalues at the TRIM points are identical to those of Fig. 5.3(a), and again every "red" band has a inversion-partner "blue" band. But the situation is clearly very different from Fig. 5.3(a): in going from 0 to π/a the Fermi energy must necessarily cross 1 point: by modifying the bands you can transform that 1 into 3, but never into 2 or 0. This is so because, essentially, the 4 edge bands "pair-up" in two separate sets of 2 bands in Fig. 5.3(a), while the 4 are inter-twined in an inextricable fashion in Fig. 5.3(b). The two situations are topologically distinct in an *even-odd* way, hence one talks about a Z_2 index.

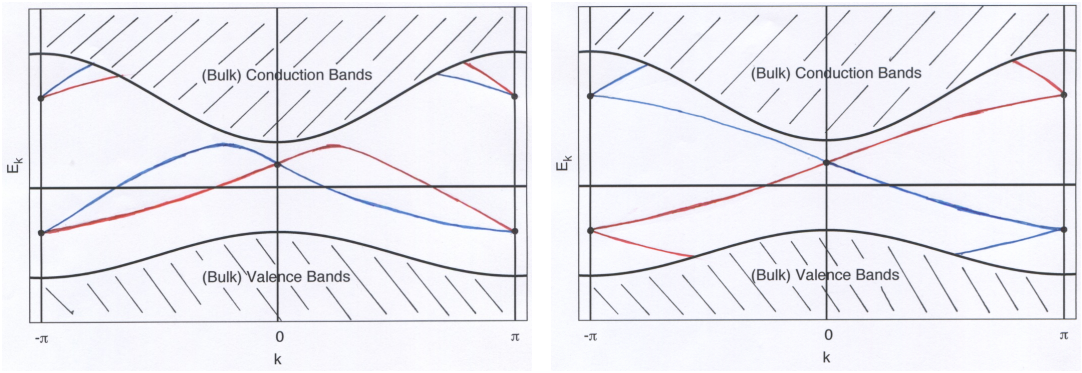

Figure 5.3.: Schematic sketch of edge states within a bulk gap. TRIM are here projected onto $k_y = \pm\pi/a$ and $k_y = 0$, and denoted by solid circles. Red and blue edge states are TR partners. On the left the insulator is topologically trivial: the Fermi energy cuts the bands into 2 points in the interval $[0, \pi/a]$, but a modification of the bands could change that integer to 0 or to 4. On the right, the insulator is topologically non-trivial: the Fermi energy cuts the edge bands into 1 point in the interval $[0, \pi/a]$ and there is no way we can change that into an even integer by deforming the bands.

Let us know return to the Kane-Mele graphene case. The question is the following: how can we distinguish from a *bulk calculation* which of the two edge-state situations we will end-up with? In other words, we would like to have a way to calculate the previously mentioned Z_2 index without having to perform a strip calculation which explicitly shows the shape and topology of the edge states. This is what Kane and Mele propose in Ref. [22]. Let us call $|u_i(\mathbf{k})\rangle$ the periodic part of the Bloch states at momentum $\mathbf{k}$ for all the occupied valence bands, labelled by i. In the present graphene case, the bands are $N_b = 2$, but in general, we will have an even number of bands, due to spin and spin-orbit coupling. Consider the matrix $m_{ij}(\mathbf{k})$ so defined:

$$m_{ij}(\mathbf{k}) = \langle u_i(\mathbf{k}) | \hat{T}_R u_j(\mathbf{k}) \rangle \qquad i, j \in 1 \cdots N_b \,, \tag{5.25}$$

which is here 2×2 (in general $N_b \times N_b$, with N_b even). Let us show that this matrix is necessarily *anti-symmetric*, due to TR-invariance. Indeed, remember that the anti-unitary nature of $\hat{T}_R$ implies that, for any two states in the Hilbert space one can write $\langle \psi_1 | \psi_2 \rangle = \langle \hat{T}_R \psi_2 | \hat{T}_R \psi_1 \rangle$. Hence:

$$\begin{aligned} m_{ij}(\mathbf{k}) &= \langle u_i(\mathbf{k}) | \hat{T}_R u_j(\mathbf{k}) \rangle \\ &= \langle \hat{T}_R \hat{T}_R u_j(\mathbf{k}) | \hat{T}_R u_i(\mathbf{k}) \rangle \\ &= -\langle u_j(\mathbf{k}) | \hat{T}_R u_i(\mathbf{k}) \rangle = -m_{ji}(\mathbf{k}) \,, \end{aligned} \tag{5.26}$$

where we used the fact that $\hat{T}_R^2 = -\mathbb{1}$ for fermions. Now, any even-dimensional anti-symmetric matrix has an associated *Pfaffian* which is defined in the following way. If $\mathbf{Z}$ denotes a $2n \times 2n$

anti-symmetric matrix, we have:

$$\begin{aligned}\mathrm{Pf}\,[\mathbf{Z}]_{2n\times 2n} &= \mathrm{Pf}\begin{bmatrix} 0 & Z_{\mu_1\mu_2} & Z_{\mu_1\mu_3} & \cdots & Z_{\mu_1\mu_{2n}} \\ Z_{\mu_2\mu_1} & 0 & Z_{\mu_2\mu_3} & \cdots & Z_{\mu_2\mu_{2n}} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ Z_{\mu_{2n}\mu_1} & Z_{\mu_{2n}\mu_2} & Z_{\mu_{2n}\mu_3} & \cdots & 0 \end{bmatrix} \\ &\stackrel{def}{=} \sum_P (-1)^P \underbrace{Z_{\mu_{P_1}\mu_{P_2}} Z_{\mu_{P_3}\mu_{P_4}} \cdots Z_{\mu_{P_{2n-1}}\mu_{P_{2n}}}}_{n \text{ factors}} , \end{aligned} \tag{5.27}$$

where the sum over P denotes the usual sum over all *permutations* of the $2n$ indices $\mu_1 \cdots \mu_{2n}$. Notice that the Pfaffian is really defined by a sum [5] which contains n products of $\mathbf{Z}$-matrix elements, and not $2n$, as the familiar $\det[\mathbf{Z}]_{2n\times 2n}$. However, a remarkable identity exists (see the book by McCoy) which links the two objects: [6]

$$\begin{aligned}\det[\mathbf{Z}]_{2n\times 2n} &= \sum_P (-1)^P \underbrace{Z_{\mu_1\mu_{P_1}} Z_{\mu_2\mu_{P_2}} \cdots Z_{\mu_{2n}\mu_{P_{2n}}}}_{2n \text{ factors}} \\ &= \left(\mathrm{Pf}\,[\mathbf{Z}]_{2n\times 2n}\right)^2 . \end{aligned} \tag{5.28}$$

In the present 2×2 case the situation is very simple, since we must have:

$$m_{ij}(\mathbf{k}) = \begin{bmatrix} 0 & P(\mathbf{k}) \\ -P(\mathbf{k}) & 0 \end{bmatrix} , \tag{5.29}$$

where $P(\mathbf{k}) = \mathrm{Pf}[m(\mathbf{k})]$, while $\det[m(\mathbf{k})] = P^2(\mathbf{k})$.

Now consider any of the TRIM $\mathbf{k}$-points: There the two states $|u_1(\mathbf{k})\rangle$ and $|u_2(\mathbf{k})\rangle$ must be TR-partners. Up to a choice of phase, you can define $e^{i\phi_{\mathbf{k}}}|u_1(\mathbf{k})\rangle = \hat{T}_R|u_2(\mathbf{k})\rangle$, hence $P(\mathbf{k}) = e^{i\phi_{\mathbf{k}}}$ and $|P(\mathbf{k})| = 1$ at all 4 TRIM $\mathbf{k}$-points. Question: can we make a smooth choice for the phase of all states such that $|P(\mathbf{k})|$ never vanishes for all $\mathbf{k} \in$ BZ? The answer is: yes if the insulator is topologically trivial, no if it is non-trivial. More in general, Kane and Mele argue that the number of zeroes that $P(\mathbf{k})$ shows in *half* of the BZ — BZ_+ so defined such that $\mathbf{k}$ and $-\mathbf{k}$ are never both contained — is a Z_2 invariant — even in the trivial case, odd in the non-trivial one — which can be calculated by the winding number of the phase of $\log[P(k)]$ in complex plane, as $\mathbf{k}$ moves along a contour C around BZ_+:

$$I = \frac{1}{2\pi i} \oint_C d\mathbf{k} \cdot \boldsymbol{\nabla}_{\mathbf{k}} \log[P(\mathbf{k})] . \tag{5.30}$$

If you want to know more about this Z_2 story, with a more pedagogical introduction to the subject, I suggest you to read the paper by Fu and Kane [23], where the connection between the Z_2 index and the so-called *modern theory of electrical polarization* [4] is discussed.

[5] Often such a sum emerges in using Wick's theorem for fermionic systems.

[6] Notice that the link exsists only if the dimension of the anti-symmetric matrix we are considering is *even*: The determinant of an odd-dimensional anti-symmetric matrix is simply zero, while the Pfaffian is not defined.

A. Kubo formula for the conductivity

We give here a quite standard linear response theory (LRT) derivation of the Hall conductivity. The derivation (in second quantization) proceeds here for a two-dimensional system on the continuum, and in the so-called scalar potential gauge, where the electric field $\mathbf{E} = -\boldsymbol{\nabla}\phi$. Following similar steps, one could provide alternative derivations for lattice systems, and/or a vector potential gauge. So, imagine having a system of electrons described by the Hamiltonian:

$$\widehat{H}_0 = \sum_\sigma \frac{1}{2m} \int d\mathbf{x}\ \widehat{\Psi}^\dagger_\sigma(\mathbf{x}) \left(-i\hbar\boldsymbol{\nabla} + \frac{e}{c}\mathbf{A}\right)^2 \widehat{\Psi}_\sigma(\mathbf{x}) + \int d\mathbf{x}\ v(\mathbf{x})\ \hat{n}(\mathbf{x}) \ + \ (\cdots)$$

where $\widehat{\Psi}_\sigma(\mathbf{x})$ is the second-quantization field operator, i.e., the operator that destroys a particle of spin σ at position $\mathbf{x}$, $\hat{n}(\mathbf{x}) = \sum_\sigma \widehat{\Psi}^\dagger_\sigma(\mathbf{x})\widehat{\Psi}_\sigma(\mathbf{x})$ is the density operator, $v(\mathbf{x})$ is a potential that the electrons feel due to the lattice and, possibly, to impurities, while the $(\cdots)$ indicate interaction terms which we do not explicitly spell out. A vector potential $\mathbf{A}(\mathbf{x})$ has been included in the kinetic term to account for a constant-in-time magnetic field $\mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A}$. Now suppose we add an electric field $\mathbf{E}(\mathbf{x},t)$ to the system ($\mathbf{E}$ is assumed irrotational, i.e., we neglect terms due to the associated extra magnetic field, whenever $\mathbf{E}$ depends on t). In a scalar potential gauge we have $\mathbf{E} = -\boldsymbol{\nabla}\phi$, and the electric potential V_e felt by the electrons is $V_e(\mathbf{x},t) = -e\phi(\mathbf{x},t)$, in such a way that the force is $-\boldsymbol{\nabla}V_e = -e\mathbf{E}$. The Hamiltonian in presence of the field becomes:

$$\hat{H}(t) = \hat{H}_0 + \int d\mathbf{x}\ V_e(\mathbf{x},t)\ \hat{n}(\mathbf{x})\ .$$

Consider now the particle current density operator $\hat{\mathbf{j}}(\mathbf{x})$.

$$\hat{\mathbf{j}}(\mathbf{x}) = \frac{1}{2m}\sum_\sigma \left(\widehat{\Psi}^\dagger_\sigma(\mathbf{x})[\boldsymbol{\Pi}\widehat{\Psi}_\sigma(\mathbf{x})] + [\boldsymbol{\Pi}\widehat{\Psi}_\sigma(\mathbf{x})]^\dagger\widehat{\Psi}_\sigma(\mathbf{x})\right)\ , \tag{A.1}$$

where $\boldsymbol{\Pi} = -i\hbar\boldsymbol{\nabla} + (e/c)\mathbf{A}$ denotes the momentum modified by the field (related to the classical velocity times the mass), which also appears in the kinetic term of the Hamiltonian.

The standard tool of linear response theory (LRT) will tell us how the averages of different operators are modified by the inclusion of the electric field term, to linear order in the field. Let me state the general result of LRT. Assuming the system, initially prepared (for instance at time $t = 0$) in a mixed state represented by a canonical (or grand-canonical) density matrix $\hat{\rho}_0 = e^{-\beta\hat{H}_0}/Z$, with $Z = \mathrm{Tr}e^{-\beta\hat{H}_0}$, with $\beta = 1/(k_BT)$, is then evolved "unitarily" under the action of $\widehat{H}(t) = \widehat{H}_0 + \int d\mathbf{x}\ \widehat{A}(\mathbf{x})a(\mathbf{x},t)$, the expectation value of an operator $\widehat{B}(\mathbf{x})$ will be modified, to linear order in the perturbing field $a(\mathbf{x},t)$, as:

$$\langle\widehat{B}(\mathbf{x})\rangle_{\mathrm{ext}}(t) = \langle\widehat{B}(\mathbf{x})\rangle_0 + \int d\mathbf{x}' \int dt'\ \chi^R_{BA}(\mathbf{x},\mathbf{x}';t-t')\ a(\mathbf{x}',t')\ , \tag{A.2}$$

where, here and henceforth, $\langle(\cdots)\rangle_0 = \mathrm{Tr}[\hat{\rho}_0(\cdots)]$, and the so-called *retarded response function* χ^R_{BA} is given by the Kubo expression:

$$\begin{aligned}
\chi^R_{BA}(\mathbf{x},\mathbf{x}';t-t') &= -\frac{i}{\hbar}\theta(t-t')\mathrm{Tr}\Big(\hat{\rho}_0[\widehat{B}_H(\mathbf{x},t),\widehat{A}_H(\mathbf{x}',t')]\Big) \\
&= -\frac{i}{\hbar}\theta(t-t')\mathrm{Tr}\Big(\hat{\rho}_0[\widehat{B}_H(\mathbf{x},t-t'),\widehat{A}_H(\mathbf{x}',0)]\Big) \\
&= \frac{i}{\hbar}\theta(t-t')\mathrm{Tr}\Big([\hat{\rho}_0,\widehat{A}_H(\mathbf{x}',0)]\widehat{B}_H(\mathbf{x},t-t')\Big) \\
&= -\theta(t-t')\int_0^\beta d\lambda\ \mathrm{Tr}\Big(\hat{\rho}_0\ \dot{A}_H(\mathbf{x}',-i\hbar\lambda)\ \widehat{B}_H(\mathbf{x},t-t')\Big)\ . \qquad \text{(A.3)}
\end{aligned}$$

The second and third form of the expression for χ^R_{BA} are simply obtained by using the cyclic property of the trace: the second explicitly shows that the response function depends only on the time difference $t-t'$; the third is particularly useful as a step towards the final form, which is based on the following identity discovered by Kubo. If we denote by $\widehat{A}_H(z) = e^{iz\hat{H}_0/\hbar}\widehat{A}e^{-iz\hat{H}_0/\hbar}$ the Heisenberg operator for general complex z, obeying the Heisenberg equation:

$$\dot{A}_H(z) \stackrel{def}{=} \frac{d}{dz}\widehat{A}_H(z) = \frac{1}{i\hbar}[\widehat{A}_H(z),\widehat{H}_0]\ , \qquad \text{(A.4)}$$

then, a simple calculation [1] shows that:

$$[\hat{\rho}_0,\widehat{A}_H(0)] = -\int_0^{-i\hbar\beta} dz\ \hat{\rho}_0\ \dot{A}_H(z) = i\hbar\int_0^\beta d\lambda\ \hat{\rho}_0\ \dot{A}_H(-i\hbar\lambda)\ . \qquad \text{(A.5)}$$

This final form of the Kubo expression is particularly useful because it will allow us to transform a current-number response function χ_{jn} into an object involving two current operators. Applying this machinery to the average current at position $\mathbf{x}$ in presence of the electric potential V_e we get:

$$\langle\hat{\mathbf{j}}(\mathbf{x})\rangle_{\mathrm{ext}}(t) = \langle\hat{\mathbf{j}}(\mathbf{x})\rangle_0 + \int d\mathbf{x}'\int dt'\ \chi^R_{\mathbf{j}n}(\mathbf{x},\mathbf{x}';t-t')\ V_e(\mathbf{x}',t')\ , \qquad \text{(A.6)}$$

where, using the final form of $\chi^R_{\mathbf{j}n}$ as indicated in Eq. (A.3) we can write:

$$\chi^R_{\mathbf{j}n}(\mathbf{x},\mathbf{x}';t-t') = -\theta(t-t')\int_0^\beta d\lambda\ \mathrm{Tr}\Big(\hat{\rho}_0\ \dot{n}_H(\mathbf{x}',-i\hbar\lambda)\ \hat{\mathbf{j}}_H(\mathbf{x},t-t')\Big)\ . \qquad \text{(A.7)}$$

We now use the continuity equation to express $\dot{n}$ in terms of $-\boldsymbol{\nabla}\cdot\mathbf{j}$. Omitting from now on the subscript H in the Heisenberg operators, and working with Cartesian components, we write:

$$\begin{aligned}
\chi^R_{\mathrm{j}_\mu n}(\mathbf{x},\mathbf{x}';t-t') &= \theta(t-t')\int_0^\beta d\lambda\ \mathrm{Tr}\Big(\hat{\rho}_0\ \boldsymbol{\nabla}_{\mathbf{x}'}\cdot\mathbf{j}(\mathbf{x}',-i\hbar\lambda)\ \hat{\mathrm{j}}_\mu(\mathbf{x},t-t')\Big) \\
&= \sum_\nu \frac{\partial}{\partial x'_\nu}\Big[\theta(t-t')\int_0^\beta d\lambda\ \langle\mathrm{j}_\nu(\mathbf{x}',-i\hbar\lambda)\mathrm{j}_\mu(\mathbf{x},t-t')\rangle_0\Big]\ . \qquad \text{(A.8)}
\end{aligned}$$

[1] Just observe that

$$-\int_0^{-i\hbar\beta} dz\ \hat{\rho}_0\ \dot{A}_H(z) = \hat{\rho}_0\ A_H(0) - \hat{\rho}_0\ A_H(-i\hbar\beta)\ ,$$

and notice that

$$\hat{\rho}_0\ A_H(-i\hbar\beta) = A_H(0)\hat{\rho}_0\ .$$

Therefore, integrating by parts (assuming the surface term infinitely far away gives no contribution) we can rewrite the average current in terms of $\boldsymbol{\nabla}_{\mathbf{x}} V_e = e\mathbf{E}$, as:

$$\langle \hat{\mathrm{j}}_\mu(\mathbf{x})\rangle_{\rm ext}(t) - \langle \hat{\mathrm{j}}_\mu(\mathbf{x})\rangle_0 = -e\int d\mathbf{x}' \int dt' \sum_\nu \Big[\theta(t-t') \int_0^\beta d\lambda \, \langle \hat{\mathrm{j}}_\nu(\mathbf{x}', -i\hbar\lambda)\hat{\mathrm{j}}_\mu(\mathbf{x}, t-t')\rangle_0\Big] \, E_\nu(\mathbf{x}', t') \; .$$

So far, everything was quite general. Now we specify our goal: we want the average (over space) extra current induced by a uniform and constant-in-time electric field $\mathbf{E}$ turned on at $t = 0$. So, we define the average field-induced electric current (accounting for the factor $-e$) as:

$$\mathrm{j}^e_\mu(t) = -e \int \frac{d\mathbf{x}}{\text{Area}} \Big(\langle \hat{\mathrm{j}}_\mu(\mathbf{x})\rangle_{\rm ext}(t) - \langle \hat{\mathrm{j}}_\mu(\mathbf{x})\rangle_0 \Big) \; . \tag{A.9}$$

We also introduce the total current operator $\widehat{\mathrm{J}}_\mu = \int d\mathbf{x} \, \hat{\mathrm{j}}_\mu(\mathbf{x})$, and notice that the total current in absence of external field actually vanishes $\langle \widehat{\mathrm{J}}_\mu\rangle_0 = 0$. Accounting for the factor $(-e)$, we get:

$$\begin{aligned} \mathrm{j}^e_\mu(t) &= \sum_\nu \sigma_{\mu\nu}(t) \, E_\nu \\ \sigma_{\mu\nu}(t) &= \frac{e^2}{\text{Area}} \int_0^t dt' \int_0^\beta d\lambda \, \langle \widehat{\mathrm{J}}_\nu(-i\hbar\lambda)\widehat{\mathrm{J}}_\mu(t-t')\rangle_0 \; . \end{aligned} \tag{A.10}$$

Now, before carrying out the integrals, let us assume the less ambitious goal of calculating $\sigma_{\mu\nu}$ for a *non-interacting* system, where in principle one can work with single-particle eigenstates $\{\phi_\alpha(\mathbf{x}) = \langle \mathbf{x}|\alpha\rangle\}$ of the Hamiltonian and associated creation operators $c^\dagger_\alpha$, in terms of which:

$$\widehat{H}_0 = \sum_\alpha \epsilon_\alpha \hat{c}^\dagger_\alpha \hat{c}_\alpha \; , \tag{A.11}$$

ϵ_α being the energy of the eigenstate measured from the chemical potential ε_F. In the same basis, expanding the field operators in terms of the $\hat{c}_\alpha$, we can express the total current as:

$$\begin{aligned} \widehat{\mathrm{J}}_\mu &= \sum_{\alpha,\beta} (\mathrm{J}_\mu)_{\alpha\beta} \hat{c}^\dagger_\alpha \hat{c}_\beta \\ (\mathrm{J}_\mu)_{\alpha\beta} &= \frac{1}{2m} \int d\mathbf{x} \Big[\phi^*_\alpha(\mathbf{x}) [\Pi_\mu \phi_\beta(\mathbf{x})] + [\Pi_\mu \phi_\alpha(\mathbf{x})]^* \phi_\beta(\mathbf{x}) \Big] = \frac{1}{m} \langle \alpha | \Pi_\mu | \beta \rangle \; , \end{aligned} \tag{A.12}$$

where, in the last step, we have used the fact that Π_μ is Hermitean. [2] The Heisenberg operators for the currents have a very simple form:

$$\begin{aligned} \widehat{\mathrm{J}}_\mu(t-t') &= \sum_{\alpha,\beta} (\mathrm{J}_\mu)_{\alpha\beta} \, e^{i(\epsilon_\alpha - \epsilon_\beta)(t-t')/\hbar} \, \hat{c}^\dagger_\alpha \hat{c}_\beta \\ \widehat{\mathrm{J}}_\nu(-i\hbar\lambda) &= \sum_{\alpha',\beta'} (\mathrm{J}_\nu)_{\alpha'\beta'} \, e^{(\epsilon_{\alpha'} - \epsilon_{\beta'})\lambda} \, \hat{c}^\dagger_{\alpha'} \hat{c}_{\beta'} \; . \end{aligned} \tag{A.13}$$

The last ingredient we need is the average over the grand-canonical ensemble of four operators, for which we can apply Wick's theorem, obtaining:

$$\langle \hat{c}^\dagger_{\alpha'} \hat{c}_{\beta'} \hat{c}^\dagger_\alpha \hat{c}_\beta \rangle_0 = \delta_{\alpha\beta}\delta_{\alpha'\beta'} f_\alpha f_{\alpha'} + \delta_{\alpha\beta'}\delta_{\alpha'\beta} f_\beta (1 - f_\alpha) \; , \tag{A.14}$$

[2] Notice that we are using here the index β, a relative of α, not to be confused, hopefully, with the inverse temperature $\beta = 1/(k_B T)$.

where

$$f_\alpha = \langle \hat{c}^\dagger_\alpha \hat{c}_\alpha \rangle_0 = \frac{1}{e^{\beta\epsilon_\alpha}+1}$$

is the usual Fermi function. Now we are ready to express:

$$\begin{aligned}
\langle \widehat{\mathrm{J}}_\nu(-i\hbar\lambda)\widehat{\mathrm{J}}_\mu(t-t')\rangle_0 &= \sum_{\alpha\beta}\sum_{\alpha'\beta'}(\mathrm{J}_\mu)_{\alpha\beta}\,(\mathrm{J}_\nu)_{\alpha'\beta'}\,e^{i(\epsilon_\alpha-\epsilon_\beta)(t-t')/\hbar}\,e^{(\epsilon_{\alpha'}-\epsilon_{\beta'})\lambda}\,\langle \hat{c}^\dagger_{\alpha'}\hat{c}_{\beta'}\hat{c}^\dagger_\alpha\hat{c}_\beta\rangle_0 \\
&= \sum_{\alpha,\alpha'}(\mathrm{J}_\mu)_{\alpha\alpha}\,(\mathrm{J}_\nu)_{\alpha'\alpha'}f_\alpha f_{\alpha'} \\
&\quad + \sum_{\alpha\beta}(\mathrm{J}_\mu)_{\alpha\beta}\,(\mathrm{J}_\nu)_{\beta\alpha}f_\beta(1-f_\alpha)e^{i(\epsilon_\alpha-\epsilon_\beta)(t-t')/\hbar}\,e^{-(\epsilon_\alpha-\epsilon_\beta)\lambda} \\
&= \langle \widehat{\mathrm{J}}_\mu\rangle_0\langle\widehat{\mathrm{J}}_\nu\rangle_0 + \sum_\alpha(\mathrm{J}_\mu)_{\alpha\alpha}\,(\mathrm{J}_\nu)_{\alpha\alpha}f_\alpha(1-f_\alpha) \\
&\quad + \sum_{\alpha\neq\beta}(\mathrm{J}_\mu)_{\alpha\beta}\,(\mathrm{J}_\nu)_{\beta\alpha}f_\beta(1-f_\alpha)e^{i(\epsilon_\alpha-\epsilon_\beta)(t-t')/\hbar}\,e^{-(\epsilon_\alpha-\epsilon_\beta)\lambda}\,.
\end{aligned}$$

We now notice that the first term is zero because $\langle \widehat{\mathrm{J}}_\mu\rangle_0 = 0$. The second, constant in time, term vanishes if we assume that the Fermi energy ε_F: **1)** either falls in a spectral gap of width Δ, and $k_BT \ll \Delta$, in such a way that $f_\alpha(1-f_\alpha)=0$ for all the α in the sum, or **2)** ε_F falls in a region where the states are *localized* due to disorder, hence the diagonal elements of the current vanish, $(\mathrm{J}_\mu)_{\alpha\alpha}=0$, for those states for which $f_\alpha(1-f_\alpha)\neq 0$ (i.e., close to ε_F). By assuming that either of this two situations is realized, we can safely conclude that the third, time-dependent, contribution is the only remaining one. By integrating over t' and over λ this third term we are left with:

$$\begin{aligned}
\int_0^t dt' \int_0^\beta d\lambda\,\langle \widehat{\mathrm{J}}_\nu(-i\hbar\lambda)\widehat{\mathrm{J}}_\mu(t-t')\rangle_0 &= -i\hbar\sum_{\alpha\neq\beta}\frac{(\mathrm{J}_\mu)_{\alpha\beta}\,(\mathrm{J}_\nu)_{\beta\alpha}}{(\epsilon_\alpha-\epsilon_\beta)^2}f_\beta(1-f_\alpha) \\
&\qquad [e^{-(\epsilon_\alpha-\epsilon_\beta)\beta}-1][1-e^{i(\epsilon_\alpha-\epsilon_\beta)t/\hbar}]\,.
\end{aligned}$$

Now, observe that:

$$f_\beta(1-f_\alpha)[e^{-(\epsilon_\alpha-\epsilon_\beta)\beta}-1] = f_\alpha - f_\beta\,,$$

which is anti-symmetric under exchange of $\alpha \leftrightarrow \beta$. Using that antisymmetry, we can finally rewrite:

$$\begin{aligned}
\sigma_{\mu\nu}(t) &= -i\frac{e^2\hbar}{\mathrm{Area}}\sum_{\epsilon_\alpha<\varepsilon_F<\epsilon_\beta}\frac{(\mathrm{J}_\mu)_{\alpha\beta}\,(\mathrm{J}_\nu)_{\beta\alpha}-(\mathrm{J}_\nu)_{\alpha\beta}\,(\mathrm{J}_\mu)_{\beta\alpha}}{(\epsilon_\alpha-\epsilon_\beta)^2} \\
&\quad + i\frac{e^2\hbar}{\mathrm{Area}}\sum_{\alpha\neq\beta}(f_\alpha-f_\beta)\frac{(\mathrm{J}_\mu)_{\alpha\beta}\,(\mathrm{J}_\nu)_{\beta\alpha}}{(\epsilon_\alpha-\epsilon_\beta)^2}e^{i(\epsilon_\alpha-\epsilon_\beta)t/\hbar}\,.
\end{aligned}$$

Notice the two contributions: the first (important) constant term, and the second time-dependent contribution, certainly important in the initial transient (indeed, it makes $\sigma_{\mu\nu}(t=0)=0$ exactly). But, upon taking a time average, we immediately see that the contribution of the time-dependent term vanishes, and we get:

$$\boxed{\sigma_{\mu\nu} = \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau dt\,\sigma_{\mu\nu}(t) \;=\; -i\frac{e^2\hbar}{\mathrm{Area}}\sum_{\epsilon_\alpha<\varepsilon_F<\epsilon_\beta}\frac{(\mathrm{J}_\mu)_{\alpha\beta}\,(\mathrm{J}_\nu)_{\beta\alpha}-(\mathrm{J}_\nu)_{\alpha\beta}\,(\mathrm{J}_\mu)_{\beta\alpha}}{(\epsilon_\alpha-\epsilon_\beta)^2}\,.} \qquad (A.15)$$

Notice that $\sigma_{xx} = \sigma_{yy} = 0$, while only the Hall conductivity $\sigma_H = \sigma_{yx} = -\sigma_{xy} \neq 0$. This crucial expression will be at the core of our discussion on the topological nature of the conductivity in certain quantum Hall systems.

We start calculating this quantity for the Haldane model assuming PBC and then taking the thermodynamic limit. As such, the calculation is definitely a *bulk property* of the system. In Haldane's model, working with PBC, there are two bands, $\epsilon_{\mathbf{k}-}$ (completely filled) and $\epsilon_{\mathbf{k}+}$ (empty). Obviously we are assuming we are at a point where the system is *insulating*, i.e., away from the critical boundaries in the phase diagram in Fig. 4.3. The sum we have to perform runs over all $\epsilon_{\mathbf{k}-}$ (the α in the previous equation), hence over the BZ of the system, while β simply refers to the "empty state" $\epsilon_{\mathbf{k}+}$, for each $\mathbf{k}$. The crucial matrix elements appearing are just given by:

$$\langle u_{\mathbf{k}\alpha}|\mathbf{J}|u_{\mathbf{k}\beta}\rangle = \frac{1}{\hbar}\langle u_{\mathbf{k}\alpha}|\boldsymbol{\nabla}_{\mathbf{k}}\mathcal{H}|u_{\mathbf{k}\beta}\rangle \ .$$

The explicit expression for the Hall conductivity is therefore:

$$\sigma_{yx} \ = \ -i\frac{e^2}{\hbar}\frac{1}{Na^2}\sum_{\mathbf{k}}^{\mathrm{BZ}} \frac{\langle u_{\mathbf{k}-}|\partial_{k_y}\mathcal{H}|u_{\mathbf{k}+}\rangle\langle u_{\mathbf{k}+}|\partial_{k_x}\mathcal{H}|u_{\mathbf{k}-}\rangle - \langle u_{\mathbf{k}-}|\partial_{k_x}\mathcal{H}|u_{\mathbf{k}+}\rangle\langle u_{\mathbf{k}+}|\partial_{k_y}\mathcal{H}|u_{\mathbf{k}-}\rangle}{(\epsilon_{\mathbf{k}-} - \epsilon_{\mathbf{k}+})^2} \ .$$

This is, at a first sight, bad news. σ_{yx} seems to depend on the band dispersion through the energy denominators, hence one might (incorrectly) believe that the result depends on band parameters such as t_1, t_2, M, etc.

However, observe that, by taking derivatives of the Schrödinger equation (see Eqs. (3.13) and (3.31)) we can easily show that:

$$\begin{aligned}
\langle u_{\mathbf{k}\alpha}|\boldsymbol{\nabla}_{\mathbf{k}}\mathcal{H}|u_{\mathbf{k}\beta}\rangle &= (\epsilon_{\mathbf{k}\alpha} - \epsilon_{\mathbf{k}\beta})\langle \boldsymbol{\nabla}_{\mathbf{k}} u_{\mathbf{k}\alpha}|u_{\mathbf{k}\beta}\rangle \\
\langle u_{\mathbf{k}\beta}|\boldsymbol{\nabla}_{\mathbf{k}}\mathcal{H}|u_{\mathbf{k}\alpha}\rangle &= (\epsilon_{\mathbf{k}\alpha} - \epsilon_{\mathbf{k}\beta})\langle u_{\mathbf{k}\beta}|\boldsymbol{\nabla}_{\mathbf{k}} u_{\mathbf{k}\alpha}\rangle \ ,
\end{aligned}$$

from which we see that the energy-denominators actually *disappear*:

$$\sigma_{yx} \ = \ i\frac{e^2}{\hbar}\frac{1}{Na^2}\sum_{\mathbf{k}}^{\mathrm{BZ}} \Big[\langle \partial_{k_x} u_{\mathbf{k}-}|u_{\mathbf{k}+}\rangle\langle u_{\mathbf{k}+}|\partial_{k_y} u_{\mathbf{k}-}\rangle - \langle \partial_{k_y} u_{\mathbf{k}-}|u_{\mathbf{k}+}\rangle\langle u_{\mathbf{k}+}|\partial_{k_x} u_{\mathbf{k}-}\rangle\Big] \ .$$

Next we notice that, in the intermediate state, we have $u_{\mathbf{k}+}$ appearing, but we can freely add a term with $u_{\mathbf{k}-}$ as well, since its contribution cancels exactly. At that point, we have reconstructed, in the intermediate state, an *identity*, $\sum_{\sigma=\pm} |u_{\mathbf{k}\sigma}\rangle\langle u_{\mathbf{k}\sigma}| = \mathbf{1}_{\mathbf{k}}$, which can easily remove.

Taking the thermodynamic limit, which transforms the sum over $\mathbf{k}$ into an integral over the whole BZ, $(Na^2)^{-1}\sum_{\mathbf{k}} \to \frac{1}{(2\pi)^2}\int d^2\mathbf{k}$, we finally write:

$$\sigma_{yx} \ = \ i\frac{e^2}{h}\frac{1}{2\pi}\int_{\mathrm{BZ}} d^2\mathbf{k} \Big[\langle \partial_{k_x} u_{\mathbf{k}-}|\partial_{k_y} u_{\mathbf{k}-}\rangle - \langle \partial_{k_y} u_{\mathbf{k}-}|\partial_{k_x} u_{\mathbf{k}-}\rangle\Big] \ . \tag{A.16}$$

Two observations are in order. First, observe that what we have done is the *undo* of the transformations done in transforming the Berry curvature into a sum over intermediate states with energy denominators. Indeed, the object we have obtained looks like an antisymmetric form closely reminiscent of a Berry curvature integrated over the whole BZ. We will see soon

that indeed it is a Berry curvature form of the spin-1/2 problem, *pulled back* into $\mathbf{k}$-space by the map $\mathbf{k} \to \mathbf{R}(\mathbf{k})$ (more about this below). Second (we stress again): the σ_{yx} just calculated in this way looks pretty much as a *bulk property*: we have used PBC and even taken the thermodynamic limit. There is no trace anywhere of the *edges* of our system, to which an experimentalist would attach contacts and leads to measure currents and voltages. More comments on this bulk-edge duality in a while.

B. $\mathbf{k}\cdot\mathbf{p}$ and envelope functions for graphite

The $\mathbf{k}\cdot\mathbf{p}$ perturbation theory, introduced in the '50s, is a classical technique of solid state band theory: it uses perturbation theory and information on the Bloch states calculated at high-symmetry points in the Brillouin Zone (BZ) to calculate the bands away from that point. A closely-related and slightly more general technique, the *envelope function theory* introduced by Luttinger and Kohn [24] in 1955, allows to tackle similar questions, with the extra bonus that you can allow for smooth *non-periodic* additional terms in the Hamiltonian. I will try to present the main ideas behind these techniques in the context of graphene, as a way to justify the tight-binding model introduced by Kane and Mele [14, 22].

Suppose you have solved the graphene band problem, in absence of spin-orbit and other relativistic effects, by finding the Bloch functions of the single-particle Hamiltonian

$$\hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{x}) \ , \tag{B.1}$$

and the corresponding bands. But suppose we have solved the problem *just* at the two Dirac points $\mathbf{K}_\pm$, i.e., we have found the *four* $E=0$ Bloch functions for the two relevant bands ($n=1,2$): [1]

$$\psi_{\mathbf{K}_\pm,n}(\mathbf{x}) = e^{i\mathbf{K}_\pm\cdot\mathbf{x}} u_{\mathbf{K}_\pm,n}(\mathbf{x}) \qquad \text{for } \ n=1,2 \ . \tag{B.2}$$

In our previous treatment of the Haldane problem we have got an approximate tight-binding description of those states, which we now recap. Denoting by $\phi_\pi(\mathbf{x}-\mathbf{r}) = \langle\mathbf{x}|\hat{c}^\dagger_{\mathbf{r}}|0\rangle$, or even more compactly as $\phi_{\mathbf{r}}(\mathbf{x})$, the $2p_z$-like π-orbital [2] centered on the Carbon atom sitting at the lattice position $\mathbf{r}$, we can form Bloch sums restricted on the two sublattices $a=A,B$ as follows:

$$\begin{aligned}
\psi_{a\mathbf{K}_\pm}(\mathbf{x}) &= \langle\mathbf{x}|\frac{e^{i\theta_{a\mathbf{K}_\pm}}}{\sqrt{N}}\sum_{\mathbf{r}_a} e^{i\mathbf{K}_\pm\cdot\mathbf{r}_a}\hat{c}^\dagger_{\mathbf{r}_a}|0\rangle = \frac{e^{i\theta_{a\mathbf{K}_\pm}}}{\sqrt{N}}\sum_{\mathbf{r}_a} e^{i\mathbf{K}_\pm\cdot\mathbf{r}_a}\phi_\pi(\mathbf{x}-\mathbf{r}_a) \\
&= e^{i\mathbf{K}_\pm\cdot\mathbf{x}}\underbrace{\frac{e^{i\theta_{a\mathbf{K}_\pm}}}{\sqrt{N}}\sum_{\mathbf{r}_a} e^{i\mathbf{K}_\pm\cdot(\mathbf{r}_a-\mathbf{x})}\phi_\pi(\mathbf{x}-\mathbf{r}_a)}_{u_{a\mathbf{K}_\pm}(\mathbf{x}) \ \text{periodic}} = e^{i\mathbf{K}_\pm\cdot\mathbf{x}}\, u_{a\mathbf{K}_\pm}(\mathbf{x}) \ .
\end{aligned} \tag{B.3}$$

Here $\mathbf{r}_{a=A(B)}$ denote the $\mathbf{r}$-sites on the $A(B)$ sublattice, respectively. Notice that we have introduced an overall phase $\theta_{a\mathbf{K}_\pm}$ whose usefulness will be appreciated in deriving the Dirac equation. The final step shows how extract the periodic part $u_{a\mathbf{K}_\pm}(\mathbf{x})$. [3] By diagonalizing

[1] We conventionally denote the energy at the Dirac point as $E=0$.

[2] Appropriately orthonormalized to the neighboring ones by the Löwdin method, or simply neglecting the small overlaps between orbitals on different sites.

[3] The proof that $u_{a\mathbf{K}_\pm}(\mathbf{x})$ are lattice-periodic is elementary.

the 2×2 tight-binding problem on this basis of Bloch-states, we can easily express the actual tight-binding Bloch eigenstates $\psi_{\mathbf{K}_\pm,n=1,2}$ in terms of $\psi_{A\mathbf{K}_\pm}$ and $\psi_{B\mathbf{K}_\pm}$. [4]

Still remaining, for simplicity, within a tight-binding two-band scheme, let us now ask how we could write a more general one-particle state $\Psi(\mathbf{x})$ using the sublattice Bloch sums $\psi_{a\mathbf{K}_\pm}$ as building blocks. To that purpose, let us introduce four smooth (see below) functions $F_{a\mathbf{K}_\pm}(\mathbf{x})$, with $a = A, B$, and construct states of the form:

$$\Psi(\mathbf{x}) = \sum_{a=A,B} \sum_{\alpha=\pm} F_{a\mathbf{K}_\alpha}(\mathbf{x})\ \psi_{a\mathbf{K}_\alpha}(\mathbf{x}) = \sum_{\mathrm{a}} F_{\mathrm{a}}(\mathbf{x})\ \psi_{\mathrm{a}}(\mathbf{x})\ , \tag{B.4}$$

where we have introduced a combined index $\mathrm{a} = a\mathbf{K}_\alpha$, running over the *four* values

$$\mathrm{a} \to (A\mathbf{K}_+, B\mathbf{K}_+, A\mathbf{K}_-, B\mathbf{K}_-)$$

to shorten the notation. The *smoothness* of the $F_{\mathrm{a}}(\mathbf{x})$ means that these functions vary very slowly on the scale of the lattice spacing $|\mathbf{a}_j|$, which in turn means that the corresponding Fourier transform

$$\hat{F}_{\mathrm{a}}(\mathbf{q}) = \int d\mathbf{x}\ e^{-i\mathbf{q}\cdot\mathbf{x}}\ F_{\mathrm{a}}(\mathbf{x})\ , \tag{B.5}$$

goes to zero very quickly, and is essentially non-vanishing only on a small region around the $\mathbf{q} = 0$ point in reciprocal space, well inside and far away from the BZ boundaries. Following Luttinger and Kohn [24], from the Bloch states $\psi_{\mathrm{a}}(\mathbf{x})$ at momentum $\mathbf{K}_\alpha$ we can easily construct Bloch states of momentum $\mathbf{K}_\alpha + \mathbf{q}$ by just adding a phase-factor $e^{i\mathbf{q}\cdot\mathbf{x}}$ in the following form:

$$\phi_{\mathbf{q},\mathrm{a}}(\mathbf{x}) = e^{i\mathbf{q}\cdot\mathbf{x}}\ \psi_{\mathrm{a}}(\mathbf{x})\ . \tag{B.6}$$

If we had *all* the Bloch-states $\psi_{n\mathbf{K}_\pm}$, at either $\mathbf{K}_+$ or $\mathbf{K}_-$, then the $\phi_{\mathbf{q},n}(\mathbf{x}) = e^{i\mathbf{q}\cdot\mathbf{x}}\ \psi_{n\mathbf{K}_\alpha}(\mathbf{x})$ so constructed would form a complete orthonormal basis in the Hilbert space [24]; since we have only two states, this will necessarily lead to a truncation of the Hilbert space, hence to an approximate scheme. Nevertheless, the functions $\phi_{\mathbf{q}\mathrm{a}} = \phi_{\mathbf{q},a\mathbf{K}_\alpha}$ are orthonormal [24],

$$\langle \phi_{\mathbf{q}'\mathrm{a}'} | \phi_{\mathbf{q}\mathrm{a}} \rangle = (2\pi)^3 \delta(\mathbf{q}' - \mathbf{q}) \delta_{\mathrm{a}',\mathrm{a}}\ ,$$

hence we can conveniently re-express $\Psi(\mathbf{x})$ as:

$$\Psi(\mathbf{x}) = \sum_{\mathrm{a}} \Big[\int \frac{d\mathbf{q}}{(2\pi)^3}\ \hat{F}_{\mathrm{a}}(\mathbf{q})\ e^{i\mathbf{q}\cdot\mathbf{x}} \Big]\ \psi_{\mathrm{a}}(\mathbf{x}) = \sum_{\mathrm{a}} \int \frac{d\mathbf{q}}{(2\pi)^3}\ \hat{F}_{\mathrm{a}}(\mathbf{q})\ \phi_{\mathbf{q}\mathrm{a}}(\mathbf{x})\ . \tag{B.7}$$

Suppose now that the Hamiltonian includes an extra term, $\hat{H} = \hat{H}_0 + \hat{H}_1$, where $\hat{H}_1$ can be either an extra potential $V_{\mathrm{ext}}(\mathbf{x})$ or a *spin-orbit term* of the form

$$\hat{V}_{\mathrm{SO}} = \frac{e\hbar}{2m^2c^2} \hat{\mathbf{S}} \cdot (\mathbf{E} \times \hat{\mathbf{p}}) = \frac{\hbar}{2m^2c^2} \hat{\mathbf{S}} \cdot (\boldsymbol{\nabla} V \times \hat{\mathbf{p}})\ , \tag{B.8}$$

or, in case there is an electric field in the z-direction, $\mathbf{E} = E_z \hat{\mathbf{z}}$, due to asymmetry or a substrate, a similar *Rashba spin-orbit term*:

$$\hat{V}_{\mathrm{R}} = \frac{e\hbar}{2m^2c^2} \hat{\mathbf{S}} \cdot (\mathbf{E} \times \hat{\mathbf{p}}) = \frac{e\hbar}{2m^2c^2} E_z\ \hat{\mathbf{z}} \cdot (\hat{\mathbf{p}} \times \hat{\mathbf{S}})\ . \tag{B.9}$$

[4] I believe it is not difficult to show, probably through a detour via the Wannier functions, that the opposite is also true: if you are given the exact band-theory Bloch eigenstates $\psi_{\mathbf{K}_\pm,n=1,2}$, then you can construct appropriate combinations $\psi_{a\mathbf{K}_\pm}$ which "approximately live" on each of the two sublattice $a = A, B$.

In all these cases, to set-up the Schrödinger equation on the (truncated) basis of the $|\phi_{\mathbf{q}\mathrm{a}}\rangle$, we should calculate matrix elements between such states. In Fourier space, we would have $\hat{H}\Psi(\mathbf{x}) = E\Psi(\mathbf{x})$ to read:

$$\sum_{\mathrm{a}'} \int \frac{d\mathbf{q}'}{(2\pi)^3} \, \langle \phi_{\mathbf{q}\mathrm{a}} | \hat{H}_0 + \hat{H}_1 | \phi_{\mathbf{q}'\mathrm{a}'} \rangle \, \hat{F}_{\mathrm{a}'}(\mathbf{q}') = E \, \hat{F}_{\mathrm{a}}(\mathbf{q}) \; . \tag{B.10}$$

And here the observation that Kane made to set-up the traditional $\mathbf{k}\cdot\mathbf{p}$ perturbation approach comes into help. Indeed, as we have noticed several times, it is immediate to show that:

$$\hat{\mathbf{p}} \, e^{i\mathbf{q}\cdot\mathbf{x}} \, \psi_{\mathrm{a}}(\mathbf{x}) = e^{i\mathbf{q}\cdot\mathbf{x}} \, (\hat{\mathbf{p}} + \hbar\mathbf{q}) \, \psi_{\mathrm{a}}(\mathbf{x}) \; , \tag{B.11}$$

which immediately implies, since $\phi_{\mathbf{q}\mathrm{a}}(\mathbf{x}) = e^{i\mathbf{q}\cdot\mathbf{x}}\psi_{\mathrm{a}}(\mathbf{x})$, that:

$$\hat{H}_0 \, \phi_{\mathbf{q}\mathrm{a}}(\mathbf{x}) = e^{i\mathbf{q}\cdot\mathbf{x}} \left[\hat{H}_0 + \frac{\hbar}{m}\mathbf{q}\cdot\hat{\mathbf{p}} + \frac{\hbar^2\mathbf{q}^2}{2m} \right] \psi_{\mathrm{a}}(\mathbf{x}) \; . \tag{B.12}$$

In essence, we can calculate all matrix elements by acting only on the $\psi_{\mathrm{a}}(\mathbf{x})$ if we remember to substitute all $\hat{\mathbf{p}} \to \hat{\mathbf{p}} + \hbar\mathbf{q}$. For instance, for the spin-orbit term we would have:

$$\hat{V}_{\mathrm{SO}} \, \phi_{\mathbf{q}\mathrm{a}}(\mathbf{x}) = e^{i\mathbf{q}\cdot\mathbf{x}} \left[\hat{V}_{\mathrm{SO}} + \frac{\hbar^2}{2m^2c^2} \hat{\mathbf{S}} \cdot (\boldsymbol{\nabla} V \times \mathbf{q}) \right] \psi_{\mathrm{a}}(\mathbf{x}) \; , \tag{B.13}$$

and similarly for the Rashba term. The relevant matrix elements of $\hat{H}_0$ are:

$$\begin{aligned} \langle \phi_{\mathbf{q}\mathrm{a}} | \hat{H}_0 | \phi_{\mathbf{q}'\mathrm{a}'} \rangle &= (2\pi)^3 \delta(\mathbf{q}' - \mathbf{q}) \, \langle \psi_{\mathrm{a}} \Big| \left[\hat{H}_0 + \frac{\hbar}{m}\mathbf{q}\cdot\hat{\mathbf{p}} + \frac{\hbar^2\mathbf{q}^2}{2m} \right] \Big| \psi_{\mathrm{a}'} \rangle \\ &= (2\pi)^3 \delta(\mathbf{q}' - \mathbf{q}) \left[\frac{\hbar}{m}\mathbf{q} \cdot \langle \psi_{\mathrm{a}} | \hat{\mathbf{p}} | \psi_{\mathrm{a}'} \rangle + \frac{\hbar^2\mathbf{q}^2}{2m} \delta_{\mathrm{a},\mathrm{a}'} \right] . \end{aligned} \tag{B.14}$$

For the ordinary spin-orbit term we would need:

$$\langle \phi_{\mathbf{q}\mathrm{a}} | \hat{V}_{\mathrm{SO}} | \phi_{\mathbf{q}'\mathrm{a}'} \rangle = \frac{\hbar}{2m^2c^2} \langle \psi_{\mathrm{a}} | e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{x}} \left[\hat{\mathbf{S}} \cdot (\boldsymbol{\nabla} V \times \hat{\mathbf{p}}) + \hat{\mathbf{S}} \cdot (\boldsymbol{\nabla} V \times \mathbf{q}) \right] | \psi_{\mathrm{a}'} \rangle \; , \tag{B.15}$$

where the first term (provided it is non-vanishing by symmetry) dominates over the second for small enough $\mathbf{q}$.

B.1. Emergence of the Dirac equation

As a warm-up exercise, let us consider the case in which there is no perturbation whatsoever, and we have just $\hat{H}_0$. Then, keeping only terms of *first order* in $\mathbf{q}$ and neglecting the second-order term $\frac{\hbar^2\mathbf{q}^2}{2m}$ we would have to solve:

$$\sum_{\mathrm{a}'} \frac{\hbar}{m}\mathbf{q} \cdot \left[\langle \psi_{\mathrm{a}} | \hat{\mathbf{p}} | \psi_{\mathrm{a}'} \rangle \right] \hat{F}_{\mathrm{a}'}(\mathbf{q}) \simeq E \, \hat{F}_{\mathrm{a}}(\mathbf{q}) \; . \tag{B.16}$$

Crucial to the whole story are therefore the matrix elements of the momentum operator $\hat{\mathbf{p}}$ in the basis of the four degenerate states $|\psi_{\mathrm{a}}\rangle$ at the two Dirac points. Symmetry arguments constrain the form of these matrix elements. For simplicity of argumentation, we will assume

that $|\psi_{\rm a}\rangle$ is given by the tight-binding expression (B.3). Notice first that $\phi_\pi(\mathbf{x}-\mathbf{r}_a) = \phi_{\mathbf{r}_a}(\mathbf{x})$, the π-orbital centered at Carbon site $\mathbf{r}_a$ is *odd* under the mirror symmetry $z \to -z$, hence:

$$\langle \phi_{\mathbf{r}_a} | \hat{p}_z | \phi_{\mathbf{r}'_a} \rangle = 0 \quad \Longrightarrow \quad \langle \psi_{\rm a} | \hat{p}_z | \psi_{\rm a'} \rangle = 0 \; . \tag{B.17}$$

We can therefore concentrate on x and y components only. Consider now the nearest-neighbor AB-bond $\mathbf{r}_A \to \mathbf{r}_A + \mathbf{d}_3$, which is along the x-axis, and the next-nearest-neighbor AA-bond $\mathbf{r}_A \to \mathbf{r}_A + \mathbf{a}_3$, which is along the y-axis. Therefore, by parity conservation [5] you immediately conclude that $\langle \phi_{\mathbf{r}_A+\mathbf{d}_3} | \hat{p}_y | \phi_{\mathbf{r}_A} \rangle = 0$ and $\langle \phi_{\mathbf{r}_A+\mathbf{a}_3} | \hat{p}_x | \phi_{\mathbf{r}_A} \rangle = 0$. The other two components are generally different from zero, and we can write, using a vector notation: $\langle \phi_{\mathbf{r}_A+\mathbf{d}_3} | \hat{\mathbf{p}} | \phi_{\mathbf{r}_A} \rangle = i\hbar\overline{k}_1 \mathbf{d}_3$ and $\langle \phi_{\mathbf{r}_A+\mathbf{a}_3} | \hat{\mathbf{p}} | \phi_{\mathbf{r}_A} \rangle = i\hbar\overline{k}_2 \mathbf{a}_3$, where the real constants $\overline{k}_{1,2}$ have dimensions of a wave-vector and simply come from performing the appropriate integrals. At this point *rotational symmetry* by $\pm 2\pi/3$ around the z-axis comes into help, and you immediately conclude that more generally:

$$\langle \phi_{\mathbf{r}_A+\mathbf{d}_j} | \hat{\mathbf{p}} | \phi_{\mathbf{r}_A} \rangle = i\hbar\overline{k}_1 \mathbf{d}_j \quad \text{and} \quad \langle \phi_{\mathbf{r}_A+\mathbf{a}_j} | \hat{\mathbf{p}} | \phi_{\mathbf{r}_A} \rangle = i\hbar\overline{k}_2 \mathbf{a}_j \; . \tag{B.18}$$

We can safely assume that no further-neighbor matrix elements of $\hat{\mathbf{p}}$ are of any significance, but the conclusions we will draw are valid even if you account for such contributions. Now we have to perform the Bloch sums of these matrix elements. Consider, for definiteness, $\langle \psi_{B\mathbf{K}_\pm} | \hat{\mathbf{p}} | \psi_{A\mathbf{K}_\pm} \rangle$, i.e., the matrix element at the *same* Dirac point, either $\mathbf{K}_+$ or $\mathbf{K}_-$, but between *opposite* sublattices. You can write it as:

$$\begin{aligned}
\langle \psi_{B\mathbf{K}_\pm} | \hat{\mathbf{p}} | \psi_{A\mathbf{K}_\pm} \rangle &= \frac{1}{N} \sum_{\mathbf{r}_A} \sum_{\mathbf{d}_j} e^{i(\theta_{A\mathbf{K}_\pm} - \theta_{B\mathbf{K}_\pm})} e^{-i\mathbf{K}_\pm \cdot \mathbf{d}_j} \langle \phi_{\mathbf{r}_A+\mathbf{d}_j} | \hat{\mathbf{p}} | \phi_{\mathbf{r}_A} \rangle \\
&= i\hbar\overline{k}_1 e^{i(\theta_{A\mathbf{K}_\pm} - \theta_{B\mathbf{K}_\pm})} \sum_{\mathbf{d}_j} e^{-i\mathbf{K}_\pm \cdot \mathbf{d}_j} \mathbf{d}_j \\
&= i\hbar\overline{k}_1 e^{i(\theta_{A\mathbf{K}_\pm} - \theta_{B\mathbf{K}_\pm})} \frac{3}{2} e^{-i\pi/3} \begin{pmatrix} 1 \\ \mp i \\ 0 \end{pmatrix} \longrightarrow \frac{3\hbar\overline{k}_1}{2} \begin{pmatrix} 1 \\ \mp i \\ 0 \end{pmatrix} \; ,
\end{aligned} \tag{B.19}$$

where the crucial point in the calculation is that $\mathbf{K}_+ \cdot \mathbf{d}_{1,2,3} = (0, 2\pi/3, -2\pi/3)$ and $\mathbf{K}_- \cdot \mathbf{d}_{1,2,3} = (2\pi/3, 0, -2\pi/3)$. The final step shows why we insisted in allowing a phase-factor $e^{i\theta_{A/B\mathbf{K}_\pm}}$ in the Bloch states: by appropriately selecting the relative phase of A and B Bloch states you can get rid of most of the annoying phase factors! Similarly, if you consider

$$\begin{aligned}
\langle \psi_{A\mathbf{K}_\pm} | \hat{\mathbf{p}} | \psi_{A\mathbf{K}_\pm} \rangle &= \frac{1}{N} \sum_{\mathbf{r}_A} \Big(\sum_{\mathbf{a}_j} e^{-i\mathbf{K}_\pm \cdot \mathbf{a}_j} \langle \phi_{\mathbf{r}_A+\mathbf{a}_j} | \hat{\mathbf{p}} | \phi_{\mathbf{r}_A} \rangle + c.c. \Big) \\
&= i\hbar\overline{k}_2 \Big(\sum_{\mathbf{a}_j} e^{-i\mathbf{K}_\pm \cdot \mathbf{a}_j} \mathbf{a}_j \Big) + c.c. = 0 \; .
\end{aligned} \tag{B.20}$$

where the result comes immediately from the fact that $\mathbf{K}_\pm \cdot \mathbf{a}_j = \mp 2\pi/3$ for all $\mathbf{a}_j$, hence you can take the phase-factor out of the sum, and then $\sum_{\mathbf{a}_j} \mathbf{a}_j = 0$. Similar calculations show that $\langle \psi_{B\mathbf{K}_\mp} | \hat{\mathbf{p}} | \psi_{A\mathbf{K}_\pm} \rangle = 0$ and $\langle \psi_{A\mathbf{K}_\mp} | \hat{\mathbf{p}} | \psi_{A\mathbf{K}_\pm} \rangle = 0$, i.e., there are no momentum matrix

[5] You do not really require that $\phi_\pi(\mathbf{x})$ is an atomic orbital for that: it is enough that it is mirror symmetric by $x \to -x$ and $y \to -y$, both symmetries being totally compatible with the graphene honeycomb lattice.

elements coupling the two *different* Dirac points. Combining these ingredients, we can finally write the equation for $F_{\rm a}(\mathbf{q})$ as:

$$\hbar v_F \left[\begin{array}{cc|cc} 0 & q_x+iq_y & 0 & 0 \\ q_x-iq_y & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & q_x-iq_y \\ 0 & 0 & q_x+iq_y & 0 \end{array}\right] \left[\begin{array}{c} \hat{F}_1(\mathbf{q}) \\ \hat{F}_2(\mathbf{q}) \\ \hline \hat{F}_3(\mathbf{q}) \\ \hat{F}_4(\mathbf{q}) \end{array}\right] = E \left[\begin{array}{c} \hat{F}_1(\mathbf{q}) \\ \hat{F}_2(\mathbf{q}) \\ \hline \hat{F}_3(\mathbf{q}) \\ \hat{F}_4(\mathbf{q}) \end{array}\right] . \tag{B.21}$$

Here we have denoted $v_F = \frac{3\hbar\bar{k}_1}{2m}$ and

$$\mathrm{a} \to (A\mathbf{K}_+, B\mathbf{K}_+, A\mathbf{K}_-, B\mathbf{K}_-) \to (1,2,3,4) .$$

If you Fourier trasform back to real space we get that the envelope function satisfies:

$$-i\hbar v_F \left[\begin{array}{cc|cc} 0 & \partial_x+i\partial_y & 0 & 0 \\ \partial_x-i\partial_y & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & \partial_x-i\partial_y \\ 0 & 0 & \partial_x+i\partial_y & 0 \end{array}\right] \left[\begin{array}{c} F_1(\mathbf{x}) \\ F_2(\mathbf{x}) \\ \hline F_3(\mathbf{x}) \\ F_4(\mathbf{x}) \end{array}\right] = E \left[\begin{array}{c} F_1(\mathbf{x}) \\ F_2(\mathbf{x}) \\ \hline F_3(\mathbf{x}) \\ F_4(\mathbf{x}) \end{array}\right] . \tag{B.22}$$

Observe that block (12) (corresponding to $\mathbf{K}_+$) is really decoupled from block (34) ($\mathbf{K}_-$). If we introduce tha Pauli matrices $\hat{\sigma}_{x,y,z}$ acting on the sublattice index $A/B = 1,2$, and $\hat{\tau}_z$ acting on the Dirac point index $\mathbf{K}_\pm$, sometimes denoted as *valley degeneracy*, we can compactly write the previous equation as:

$$-i\hbar v_F \left[\hat{\sigma}_x\partial_x - \hat{\tau}_z\hat{\sigma}_y\partial_y\right] \mathbf{F}(\mathbf{x}) = E\, \mathbf{F}(\mathbf{x}) . \tag{B.23}$$

Equivalently, we might write this *effective mass (envelope function) Hamiltonian* in the Dirac form:

$$\mathcal{H}_0 = -i\hbar v_F \left[\hat{\sigma}_x\partial_x - \hat{\tau}_z\hat{\sigma}_y\partial_y\right] . \tag{B.24}$$

B.2. The Spin-Orbit term

As discussed in the text, we can effectively keep only the $\hat{S}_z$ spin-orbit term at low energies. As already remarked, for small $\mathbf{q}$ we can forget about the $\mathbf{q}$-dependent terms and simply take into account:

$$\langle\psi_{\rm a}|(\boldsymbol{\nabla}V\times\hat{\mathbf{p}})_z|\psi_{\rm a'}\rangle . \tag{B.25}$$

Again, let us look first at the basic matrix elements of the $\phi_{\mathbf{r}_a}(\mathbf{x})$ orbitals centered on the Carbon atoms. This time we notice that:

$$\langle\phi_{\mathbf{r}_A+\mathbf{d}_3}|\Big[(\partial_x V)\,\hat{p}_y - (\partial_y V)\,\hat{p}_x\Big]|\phi_{\mathbf{r}_A}\rangle = 0 , \tag{B.26}$$

because both terms are *odd* under $y\to -y$ aroud the $\mathbf{r}_A \to \mathbf{r}_A + \mathbf{d}_3$ bond, which is along the x axis (the first because of $\hat{p}_y$, the second because of $\partial_y V$). Rotational symmetry by $\pm 2\pi/3$ around the z-axis immediately implies that quite generally:

$$\langle\phi_{\mathbf{r}_A+\mathbf{d}_j}|(\boldsymbol{\nabla}V\times\hat{\mathbf{p}})_z|\phi_{\mathbf{r}_A}\rangle = 0 \quad\Rightarrow\quad \langle\psi_{B\mathbf{K}_\pm}|(\boldsymbol{\nabla}V\times\hat{\mathbf{p}})_z|\psi_{A\mathbf{K}_\pm}\rangle = 0 . \tag{B.27}$$

Similar conclusions apply to the inter-valley elements $\langle\psi_{B\mathbf{K}_\mp}|(\boldsymbol{\nabla}V\times\hat{\mathbf{p}})_z|\psi_{A\mathbf{K}_\pm}\rangle = 0$.

Next we consider the other relevant matrix element: $\langle\phi_{\mathbf{r}_A+\mathbf{a}_3}|(\boldsymbol{\nabla}V\times\hat{\mathbf{p}})_z|\phi_{\mathbf{r}_A}\rangle$. Here we notice that:

$$\langle\phi_{\mathbf{r}_A+\mathbf{a}_3}|\Big[(\partial_x V)\,\hat{p}_y - (\partial_y V)\,\hat{p}_x\Big]|\phi_{\mathbf{r}_A}\rangle = -i\hbar C \neq 0\,, \tag{B.28}$$

because $\partial_x V$ has *no definite parity* under $x\to -x$ around the bond $\mathbf{r}_A \to \mathbf{r}_A+\mathbf{a}_3$. Moreover, a careful look at the lattice structure shows that the *sign* of $\partial_x V$ is exactly opposite in the corresponding integral for the B-sublattice, i.e.,

$$\langle\phi_{\mathbf{r}_B+\mathbf{a}_3}|\Big[(\partial_x V)\,\hat{p}_y - (\partial_y V)\,\hat{p}_x\Big]|\phi_{\mathbf{r}_B}\rangle = +i\hbar C \neq 0\,. \tag{B.29}$$

These results, obtained for the $\mathbf{a}_3$-bond, extend by $\pm 2\pi/3$ rotational symmetry around the z-axis to all the $\mathbf{a}_j$ bonds. Summarizing, we have:

$$\langle\phi_{\mathbf{r}_B+\mathbf{a}_j}|(\boldsymbol{\nabla}V\times\hat{\mathbf{p}})_z|\phi_{\mathbf{r}_B}\rangle = -\langle\phi_{\mathbf{r}_A+\mathbf{a}_j}|(\boldsymbol{\nabla}V\times\hat{\mathbf{p}})_z|\phi_{\mathbf{r}_A}\rangle = +i\hbar C \neq 0\,. \tag{B.30}$$

At this point it is straightforward to evaluate:

$$\begin{aligned}\langle\psi_{A\mathbf{K}_\pm}|(\boldsymbol{\nabla}V\times\hat{\mathbf{p}})_z|\psi_{A\mathbf{K}_\pm}\rangle &= \frac{1}{N}\sum_{\mathbf{r}_A}\Big(\sum_{\mathbf{a}_j} e^{-i\mathbf{K}_\pm\cdot\mathbf{a}_j}\langle\phi_{\mathbf{r}_A+\mathbf{a}_j}|(\boldsymbol{\nabla}V\times\hat{\mathbf{p}})_z|\phi_{\mathbf{r}_A}\rangle + c.c.\Big)\\ &= \sum_{\mathbf{a}_j}\Big(-i\hbar C e^{-i\mathbf{K}_\pm\cdot\mathbf{a}_j} + c.c.\Big) = \pm 3\sqrt{3}\hbar C\,.\end{aligned} \tag{B.31}$$

Adding the spin-orbit term at $\mathbf{q}=0$ as a perturbation to the previous Dirac term we would write the effective mass Hamiltonian in momentum space as:

$$\left[\begin{array}{cc|cc} s\Delta_{\rm SO} & \hbar v_F(q_x+iq_y) & 0 & 0\\ \hbar v_F(q_x-iq_y) & -s\Delta_{\rm SO} & 0 & 0\\ \hline 0 & 0 & -s\Delta_{\rm SO} & \hbar v_F(q_x-iq_y)\\ 0 & 0 & \hbar v_F(q_x+iq_y) & s\Delta_{\rm SO}\end{array}\right] \tag{B.32}$$

where $s=+$ for the $\uparrow$-electrons, and $s=-$ for $\downarrow$ ones, while $\Delta_{\rm SO}$, collecting all factors, is:

$$\Delta_{\rm SO} = \frac{\hbar}{2m^2c^2}\frac{3\sqrt{3}}{2}\hbar C\,. \tag{B.33}$$

In a more compact form, we write this as:

$$\mathcal{H}(\mathbf{q}) = \mathcal{H}_0(\mathbf{q}) + \mathcal{H}_{\rm SO} = \hbar v_F\,[q_x\hat{\sigma}_x - q_y\hat{\tau}_z\hat{\sigma}_y] + \Delta_{\rm SO}\hat{s}_z\hat{\tau}_z\hat{\sigma}_z\,. \tag{B.34}$$

C. Time Reversal

The subject of Time Reversal (TR) requires a rather detailed analysis — crucial to understanding, for instance, the very definitions of Wigner-Dyson ensembles in Random Matrix Theory —, which is usually omitted in standard Quantum Mechanics classes. My notes on this topic have grown beyond the point where I decided to make a separate chapter of it. The chapter is heavily based on the treatment of TR presented by Sakurai, in *Modern Quantum Mechanics*, and Metha, in *Random Matrices*, together with the clear exposition of quaternions made by Dutra, in *Cavity Quantum Electrodynamics*. Sakurai is quite clear, but it does not give enough details for the purpose of understanding the symplectic case of Random Matrix theory. Metha is very advanced, detailed and wonderfully complete, but *alas*, at times, a bit cryptic, unless you go very patiently in the details of every paragraph.

C.1. Preliminaries

The way this topic is usually tackled is, roughly, the following. Take a spinless non-relativistic particle moving in some potential $V(\mathbf{x})$ and write its Schrödinger equation (SE) in position-representation:

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})\right]\psi(\mathbf{x},t)\ . \tag{C.1}$$

Taking the complex conjugate of the SE in Eq. C.1 and observing that the Hamiltonian is a *real* operator in position representation we can write:

$$-i\hbar\frac{\partial}{\partial t}\psi^*(\mathbf{x},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})\right]\psi^*(\mathbf{x},t)\ . \tag{C.2}$$

Consider now the wave-function $\psi_R(\mathbf{x},t) = \psi^*(\mathbf{x},-t)$. It is clear that the change of variable $t \to -t$ exactly reabsorbs the minus sign in front of the first-order time-derivative, so that $\psi_R(\mathbf{x},t)$ obeys exactly the same equation as $\psi(\mathbf{x},t)$:

$$i\hbar\frac{\partial}{\partial t}\psi_R(\mathbf{x},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})\right]\psi_R(\mathbf{x},t)\ . \tag{C.3}$$

Consider, on the other hand, the average momentum of the wave-packet $\psi_R(\mathbf{x},t)$:

$$\begin{aligned}\langle\psi_R(t)|\hat{\mathbf{p}}|\psi_R(t)\rangle &= \int d\mathbf{x}\ \psi_R^*(\mathbf{x},t)[-i\hbar\nabla]\psi_R(\mathbf{x},t) = \int d\mathbf{x}\ \psi_R(\mathbf{x},t)[+i\hbar\nabla]\psi_R^*(\mathbf{x},t)\\ &= -\int d\mathbf{x}\ \psi^*(\mathbf{x},-t)[-i\hbar\nabla]\psi(\mathbf{x},-t) = -\langle\psi(-t)|\hat{\mathbf{p}}|\psi(-t)\rangle\ .\end{aligned} \tag{C.4}$$

Here the second equality in the first line is justified by the fact that the average momentum is a real quantity coinciding with its complex conjugate. So, that average momentum of $\psi_R(\mathbf{x},t)$

is just the opposite of that of ψ at time $-t$. An entirely similar derivation shows that angular momentum, for instance, or any operator involving the imaginary unit i will change sign upon TR, while operators that are real, like position or energy, do not change sign. Evidently, an Hamiltonian like the one written above obeys TR invariance. What about, for instance, one with a magnetic field? The SE, if q is the charge of the particle and $\mathbf{A}$ the vector potential, reads:

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \left[\frac{1}{2m}\left(-i\hbar\nabla - \frac{q}{c}\mathbf{A}\right)^2 + V(\mathbf{x})\right]\psi(\mathbf{x},t)\ . \tag{C.5}$$

Evidently, we cannot take here complex conjugation without ruining the Hamiltonian, which is no-longer real! So, TR is not obeyed in presence of a magnetic field. (Indeed, we know from classical physics that if we reverse the momentum of a particle, its trajectory, in the magnetic field, curves in a different way, because the Lorentz force is reversed.)

With a movie analogy, we might picture this by saying that if TR invariance applies, we would not be able to distinguish if the movie showing the particle motion is observed in the forward direction or with the rewind button inserted: both make perfect physical sense. On the contrary, if TR is broken, the "rewind movie" makes no sense physically: particles curve in the wrong direction under the action of a Lorentz force, for instance. To provoke you a bit, think of this small apparent paradox. As you know, a wavepacket describing a free non-relativistic particle in absence of any external fields and potentials inevitably *spreads* in time. How can you make sense of this spreading in the movie-backward picture? Spreading seems to be inherently connected with an "arrow of time", but the motion of a free-particle should be the archetype of time-reversal invariance! Any clue?

What about spin? Like angular momenta, we would like spins to be reversed under TR. Consider a spin-1/2 particle. If it is in an eigenstate of S^y:

$$|\pm\rangle_y = \frac{1}{\sqrt{2}}\left[|\uparrow\rangle \pm i|\downarrow\rangle\right]\ ,$$

then evidently a simple complex conjugation will reverse the spin. But, clearly, complex conjugation is not enough to reverse the spin of an eigenstate of S^x or of S^z: we need something else. This extra piece is just a rotation by π around the y-axis in spin space, performed by $e^{i(\pi/2)\sigma_y} = i\sigma_y$. More about this, including Kramers degeneracy, below.

For the time being, we pause here and notice a small weakness of the previous approach. Consider a spinless particle moving in an harmonic potential in the presence of a uniform electric field E, so that $V(\hat{x}) = k\hat{x}^2/2 - qE\hat{x}$. In position representation the Hamiltonian is evidently still real, and we would confortably conclude (correctly) that an electric field does not break TR invariance. But if we write the SE, for some reason, in momentum representation where $\hat{x} = i\hbar\partial/\partial p$ then we would not have that the Hamiltonian is real, and we would be a bit puzzled. The crucial point we will make below, with a proper derivation, is that if a system obeys TR invariance then we can always find a representation (i.e., a basis) in which the Hamiltonian is *real* (if there are no spins or integer spins) or (do not worry if you do not understand, it will be made clear later on) *quaternion real* (if there are spins-1/2 or more generally half-integer spins). To do that, we have to formulate the problem from scratch in a more precise way.

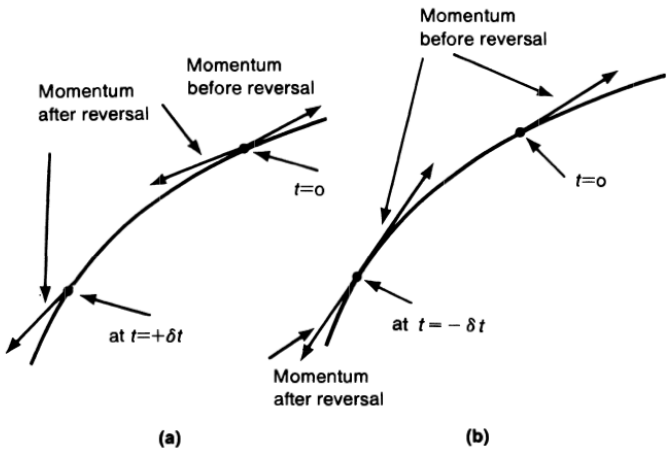

Figure C.1.: Figure taken from Sakurai's book *Modern Quantum Mechanics*, illustrating the idea behind Time Reversal (TR) invariance, with a classical-like trajectory picture. (a, Left) The TR operation (inversion of momenta/spins) is applied at time $t = 0$ to a state $|\psi\rangle$, and then the system is evolved for a time $+\delta t$: the resulting quantum state is $\hat{U}(\delta t, 0)\hat{T}_R|\psi\rangle$. (b, Right) The system is propagated backward in time, up to time $-\delta t$, and then the TR operation (inversion of momenta/spins) is applied: the resulting state is $\hat{T}_R\hat{U}(-\delta t, 0)|\psi\rangle$. The two states coincide if the system is TR-invariant.

C.2. A more precise definition of TR-invariance

So, let us abandon the idea that TR consists in reversing the time in a first-order-in-time differential equation, and let us try to define an appropriate operator $\hat{T}_R$ acting on states of the Hilbert space, and having the correct properties discussed above. The idea is the following. Take any state $|\psi\rangle$ in the Hilbert space, describing a set of particles, with their momenta and possibly with their spins, etc., at some time t_0. If we apply $\hat{T}_R$ to $|\psi\rangle$ (i.e., in some way we reverse all momenta and spins) and propagate then the state for a time interval $\delta t = t - t_0$ up to time t by applying the evolution operator $\hat{U}(t, t_0)$, we get the state $\hat{U}(t, t_0)\hat{T}_R|\psi\rangle$. Then, if the dynamics is TR-invariant, this state should coincide with that obtained by propagating backward in time by $\delta t = t - t_0$ and then applying $\hat{T}_R$, i.e., $\hat{T}_R\hat{U}(t_0 - \delta t, t_0)|\psi\rangle \equiv \hat{T}_R\hat{U}(2t_0 - t, t_0)|\psi\rangle$:

$$\hat{U}(t, t_0)\hat{T}_R|\psi\rangle = \hat{T}_R\hat{U}(2t_0 - t, t_0)|\psi\rangle \quad \forall\psi \quad \Longleftrightarrow \quad \text{TR-invariance holds .} \tag{C.6}$$

Fig. C.1 tries to give a picture illustrating the previous idea. Notice that the evolution operator $\hat{U}$ governs the dynamics, while $\hat{T}_R$ is an operator acting on *states*, which we still have to define in a way compatible with the physical picture presented above. Since the previous equality should hold for any $|\psi\rangle$, it should apply for the operators:

$$\hat{U}(t, t_0)\hat{T}_R = \hat{T}_R\hat{U}(2t_0 - t, t_0) \quad \Longleftrightarrow \quad \text{TR-invariance holds .} \tag{C.7}$$

Now take a derivative with respect to time, and recall that $\hat{U}(t, t_0)$ satisfies the usual SE we get:

$$\left(\frac{1}{i\hbar}\hat{H}(t)\hat{U}(t, t_0)\right)\hat{T}_R = \hat{T}_R\left(-\frac{1}{i\hbar}\hat{H}(2t_0 - t)\hat{U}(2t_0 - t, t_0)\right) . \tag{C.8}$$

Assume now, for the remaining part of this discussion, that $\hat{H}$ *does not depend on time*: we will go back to the time-dependent case when we will discuss time-periodic Hamiltonians and Floquet theory, see Sec. C.8. Then, taking $t = t_0 = 0$ we deduce that:

$$\left(\frac{1}{i\hbar}\hat{H}\right)\hat{T}_R = \hat{T}_R\left(-\frac{1}{i\hbar}\hat{H}\right) \qquad \Longleftrightarrow \qquad \text{TR-invariance holds .} \tag{C.9}$$

And here comes the first result: $\hat{T}_R$ *cannot be a unitary operator!* Indeed, if $\hat{T}_R$ was unitary, then we would simply cancel $1/(i\hbar)$ on both sides and conclude that $\hat{H}\hat{T}_R = -\hat{T}_R\hat{H}$, which makes no physical sense at all: it would imply that if $|n\rangle$ is an eigenstate of $\hat{H}$ with eigenvalue E_n, then $\hat{T}_R|n\rangle$ is an eigenstate with energy $-E_n$, and this would apply to arbitrarily large values of E_n. Essentially, it would imply that if the spectrum of $\hat{H}$ is unbouded from above (for instance, as in the hydrogen atom case), then $\hat{H}$ has no ground state! The way out is that $\hat{T}_R$ is an *anti-linear and anti-unitary operator.* [1] If $\hat{T}_R$ is anti-linear, then the $-1/(i\hbar)$ becomes $1/(i\hbar)$ when I move it to the left of $\hat{T}_R$ and cancels with the corresponding factor in the left-hand side, leading to:

$$\hat{H}\,\hat{T}_R = \hat{T}_R\,\hat{H} \qquad \Longleftrightarrow \qquad \text{TR-invariance holds ,} \tag{C.10}$$

which makes perfect sense: $\hat{T}_R$ commutes with $\hat{H}$ if TR-invariance holds, as any symmetry operation does.

C.3. Properties of $\hat{T}_R$

Let us abandon $\hat{H}$ for a while, and concentrate on the properties of $\hat{T}_R$. We have already met an anti-linear operator above: the complex conjugation $\hat{C}$. Its precise definition depends on the choice of the basis $\{|\alpha\rangle\}$ in the Hilbert space and is given by:

$$\hat{C}|\psi\rangle = \hat{C}\sum_\alpha \psi_\alpha|\alpha\rangle \stackrel{def}{=} \sum_\alpha \psi^*_\alpha|\alpha\rangle \; . \tag{C.11}$$

Notice that $\hat{C}$ acts, given a basis, on the wave-functions amplitudes ψ_α, transforming them to their complex conjugates, *without affecting at all the kets* $|\alpha\rangle$. Obviously $\hat{C}^2 = \mathbb{1}$, or $\hat{C} = \hat{C}^{-1}$. Now, any anti-unitary operator [2] can be written as a product of a unitary operator $\hat{K}$ times $\hat{C}$, so that:

$$\hat{T}_R = \hat{K}\hat{C} \quad \text{ with } \quad \hat{K}^\dagger\hat{K} = \hat{K}\hat{K}^\dagger = \mathbb{1} \; . \tag{C.12}$$

[1] An operator is anti-linear if $\hat{A}(\alpha\psi) = \alpha^*\hat{A}\psi$, while $\hat{A}(\psi_1+\psi_2) = \hat{A}\psi_1 + \hat{A}\psi_2$ as for linear operators. Contrary to unitary operators, which conserve the scalar product, $\langle\hat{U}\phi|\hat{U}\psi\rangle = \langle\phi|\psi\rangle$, an anti-linear operator is called anti-unitary, if $\langle\hat{A}\phi|\hat{A}\psi\rangle = \langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*$.

[2] According to the pioneering work of Wigner, symmetries in Quantum Mechanics are represented by linear operators that preserve the modulus of the scalar product:

$$|\langle\hat{U}\phi|\hat{U}\psi\rangle| = |\langle\phi|\psi\rangle| \; .$$

With a technically quite involved proof, Wigner was able to show that, apart from adjusting phase-factors, the only two physically relevant cases are that of unitary operators, and that of *anti-unitary* operators, such as time-reversal.

Since $\hat{C}$ depends on the basis we choose, so will $\hat{K}$: if you change your basis, both will be affected. If you make a unitary transformation on the states $|\psi\rangle \to \hat{U}|\psi\rangle$, [3] then all operators should be consistently changed as $\hat{A} \to \hat{U}\hat{A}\hat{U}^{-1} = \hat{U}\hat{A}\hat{U}^\dagger$ in order for scalar products and matrix elements to be unchanged. Consequently, $\hat{T}_R$ will change as:

$$\hat{T}_R = \hat{K}\hat{C} \to \hat{U}\hat{K}\hat{C}\hat{U}^\dagger = \hat{U}\hat{K}\hat{C}\hat{U}^\dagger(\hat{C}^{-1}\hat{C}) = (\hat{U}\hat{K}\hat{U}^T)\hat{C}\ , \tag{C.13}$$

where we have used that $\hat{C}\hat{U}^\dagger\hat{C}^{-1} = \hat{U}^T$ where $\hat{U}^T$ is the *transpose* of $\hat{U}$, with matrix elements $\langle\alpha'|\hat{U}^T|\alpha\rangle = \langle\alpha|\hat{U}|\alpha'\rangle$. [4] All this amounts to saying that, upon a unitary transformation of states $|\psi\rangle \to \hat{U}|\psi\rangle$, the operator $\hat{K}$ transforms as:

$$|\psi\rangle \to \hat{U}|\psi\rangle \qquad \Longrightarrow \qquad \hat{K} \to \hat{U}\hat{K}\hat{U}^T\ . \tag{C.14}$$

This is just mathematics of anti-unitary operators.

Let us now inject a bit of physics: acting *twice* with $\hat{T}_R$ we should not change the state, apart from a possible overall phase factor. Therefore:

$$\hat{T}_R^2 = e^{i\theta}\mathbb{1}\ . \tag{C.15}$$

How much can θ be will be our next point: we will soon show that $\theta = 0, \pi$ are the only two possibilities that nature allows. Indeed, $\hat{T}_R^2 = (\hat{K}\hat{C})(\hat{K}\hat{C})$ and $\hat{C}\hat{K}\hat{C} = \hat{K}^*$, [5] and therefore:

$$\hat{T}_R^2 = \hat{K}\hat{K}^* = e^{i\theta}\mathbb{1}\ . \tag{C.16}$$

But $\hat{K}$ is unitary, so that $\hat{K}\hat{K}^\dagger = \mathbb{1}$, or, by taking the complex conjugate:

$$\hat{K}^*\hat{K}^T = \mathbb{1}\ . \tag{C.17}$$

Multiply now this equation by $\hat{K}$ on the left and use $\hat{K}\hat{K}^* = e^{i\theta}\mathbb{1}$, obtaining:

$$e^{i\theta}\hat{K}^T = \hat{K}\ . \tag{C.18}$$

Now iterate the last equation by writing:

$$\hat{K} = e^{i\theta}\hat{K}^T = e^{i\theta}\left(e^{i\theta}\hat{K}^T\right)^T = e^{2i\theta}\hat{K}\ . \tag{C.19}$$

A miracle has occurred: due to the unitarity requirement for $\hat{K}$, the *a priori* generic phase $e^{i\theta}$ has to be such that $e^{2i\theta} = 1$, i.e., only the cases $\theta = 0$ or $\theta = \pi$ are allowed!

Summarizing, there are only two possible physically allowed cases:

$$\theta = 0 \iff \hat{T}_R^2 = \mathbb{1} \iff \hat{K}\hat{K}^* = \mathbb{1} \Longrightarrow \hat{K}^T = \hat{K}\ , \tag{C.20}$$

$$\theta = \pi \iff \hat{T}_R^2 = -\mathbb{1} \iff \hat{K}\hat{K}^* = -\mathbb{1} \Longrightarrow \hat{K}^T = -\hat{K}\ , \tag{C.21}$$

i.e., $\hat{K}$ is not only unitary, but it must be either symmetric (for $\theta = 0$) or antisymmetric (for $\theta = \pi$).

[3] Equivalent results are obtained by changing the basis as $|\alpha\rangle \to |\tilde{\alpha}\rangle = U^\dagger|\alpha\rangle$.

[4] The proof of this fact is elementary. Take the generic matrix element $\langle\phi|\hat{C}\hat{U}^\dagger\hat{C}^{-1}|\psi\rangle$, express $|\psi\rangle = \sum_\alpha \psi_\alpha|\alpha\rangle$ and $|\phi\rangle = \sum_{\alpha'} \phi_{\alpha'}|\alpha'\rangle$ and do the simple algebra. Equivalently, recall that $\hat{U}^\dagger = (\hat{U}^T)^*$ and that when $\hat{C}$ operates on anything but $\hat{U}^\dagger$, its effect will cancel with that of $\hat{C}^{-1}$ to the right, while the action on $\hat{U}^\dagger$ will simply give $\hat{U}^T$.

[5] Again a simple proof as above: it is enough to let $\hat{C}$ act on $\hat{K}$, because $\hat{C}^2 = \mathbb{1}$.

C.4. Transformation of operators under time-reversal

Let us now consider how matrix elements of operators are related under TR. Here a bit of caution is needed: the Dirac bra-ket notation can be confusing (it was invented to handle linear operators, rather than anti-linear ones). If we denote by $|\psi^R\rangle = \hat{T}_R|\psi\rangle$ and $|\phi^R\rangle = \hat{T}_R|\phi\rangle$ the time-reversed of two states $|\psi\rangle$ and $|\phi\rangle$, one can show that, as a consequence of the anti-unitary nature of $\hat{T}_R$, we must have: [6]

$$\langle\phi|\hat{A}|\psi\rangle = \langle\psi^R|\underbrace{\hat{T}_R\hat{A}^\dagger\hat{T}_R^{-1}}_{\stackrel{def}{=}\hat{A}^R}|\phi^R\rangle = \langle\psi^R|\hat{A}^R|\phi^R\rangle \ . \tag{C.22}$$

The operator $\hat{A}^R = \hat{T}_R\hat{A}^\dagger\hat{T}_R^{-1}$ is called the *dual* of $\hat{A}$ under TR. Using $\hat{T}_R = \hat{K}\hat{C}$, and $\hat{C}\hat{A}^\dagger\hat{C}^{-1} = \hat{A}^T$, one can easily show that:

$$\hat{A}^R = \hat{T}_R\hat{A}^\dagger\hat{T}_R^{-1} = \hat{K}\left(\hat{C}\hat{A}^\dagger\hat{C}^{-1}\right)\hat{K}^{-1} = \hat{K}\hat{A}^T\hat{K}^{-1} \ . \tag{C.23}$$

As done with parity, one can classify the observables as being *even* or *odd* under TR: since $\hat{A} = \hat{A}^\dagger$ for observables, then $\hat{A}^R = \hat{T}_R\hat{A}\hat{T}_R^{-1} = \pm\hat{A}$ for even/odd-TR observables.

Let us return to the physical case of a non-relativistic particle in elementary quantum mechanics. It is physically quite reasonable/obvious that $\hat{\mathbf{x}}$ must be even under TR,

$$\hat{\mathbf{x}}^R = \hat{T}_R\hat{\mathbf{x}}\hat{T}_R^{-1} = \hat{\mathbf{x}} \ ,$$

as a consequence of $\langle\psi|\hat{\mathbf{x}}|\psi\rangle = \langle\psi^R|\hat{\mathbf{x}}|\psi^R\rangle$. The picture in your mind might be: if I reverse all spins and momenta, the average positions do not change at all. Then you immediately deduce that, in order to preserve the canonical commutation relationships $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$, $\hat{\mathbf{p}}$ must be *odd* under TR, i.e., [7]

$$\hat{\mathbf{p}}^R = \hat{T}_R\hat{\mathbf{p}}\hat{T}_R^{-1} = -\hat{\mathbf{p}} \ .$$

Finally, in order to preserve the angular momentum commutation relations, showing a crucial imaginary unit i, $[\hat{J}_i, \hat{J}_j] = i\epsilon_{ijk}\hat{J}_k$, $\hat{\mathbf{J}}$ must be also *odd* under TR:

$$\hat{\mathbf{J}}^R = \hat{T}_R\hat{\mathbf{J}}\hat{T}_R^{-1} = -\hat{\mathbf{J}} \ ,$$

and this applies to spins, orbital angular momenta, total angular momenta: any angular momentum!

C.5. Hamiltonians invariant under time-reversal

The previous analysis is absolutely independent of $\hat{H}$, and of whether TR-invariance holds or not. Let us now look at the consequences of TR-invariance on $\hat{H}$. If TR invariance holds,

[6] The proof goes as follows. Denote by $|\chi\rangle = \hat{A}^\dagger|\phi\rangle$, and by $|\chi^R\rangle = \hat{T}_R|\chi\rangle$. Then:

$$\begin{aligned}\langle\phi|\hat{A}|\psi\rangle &= \langle\chi|\psi\rangle = \langle\psi^R|\chi^R\rangle = \langle\psi^R|\hat{T}_R\hat{A}^\dagger|\phi\rangle = \langle\psi^R|\hat{T}_R\hat{A}^\dagger\hat{T}_R^{-1}\hat{T}_R|\phi\rangle \\ &= \langle\psi^R|\hat{T}_R\hat{A}^\dagger\hat{T}_R^{-1}|\phi^R\rangle \ .\end{aligned}$$

[7] The imaginary unit and the anti-linear nature of $\hat{T}_R$ are crucial for that.

then $\hat{T}_R\hat{H} = \hat{H}\hat{T}_R$, or $\hat{T}_R\hat{H}\hat{T}_R^{-1} = \hat{H}$, or:

$$\hat{H} = \hat{T}_R\hat{H}\hat{T}_R^{-1} = \hat{K}\left(\hat{C}\hat{H}\hat{C}^{-1}\right)\hat{K}^{-1} = \hat{K}\hat{H}^T\hat{K}^{-1} = \hat{H}^R\,, \tag{C.24}$$

where we have made use of the fact that $\hat{H} = \hat{H}^\dagger$, which implies $\hat{C}\hat{H}\hat{C}^{-1} = \hat{H}^T$. So, if TR-invariance holds, we can equivalently say that $\hat{H}$ is *even* under TR, or that $\hat{H}$ is *self-dual*.

Now let us go back to the two possibilities that nature allows: $\hat{T}_R^2 = +\mathbb{1}$ (and $\hat{K}^T = \hat{K}$) or $\hat{T}_R^2 = -\mathbb{1}$ (and $\hat{K}^T = -\hat{K}$). We will see that they correspond, respectively, to the case of *integer* or *half-integer* spin/angular momentum. But before proceeding with this analysis, let us immediately point out a very deep consequence of TR-invariance in conjunction with the case $\hat{T}_R^2 = -\mathbb{1}$: it is called *Kramers degeneracy*. Indeed, take an eigenstate $|n\rangle$ of $\hat{H}$ with energy E_n and consider the TR-state $\hat{T}_R|n\rangle$. If $\hat{H}$ is TR-invariant, then it commutes with $\hat{T}_R$, which immediately implies (as you know from elementary QM) that $\hat{T}_R|n\rangle$ is also an eigenstate with the same energy E_n. The question at this point is: is perhaps $\hat{T}_R|n\rangle$ simply related to $|n\rangle$ by an overall phase factor, or it is a genuinely independent state, in which case I would have degeneracy? Let's see. Assume that $\hat{T}_R|n\rangle = e^{i\delta}|n\rangle$ and apply $\hat{T}_R$ once more. You get:

Kramers degeneracy

$$\hat{T}_R^2|n\rangle = \hat{T}_R e^{i\delta}|n\rangle = e^{-i\delta}\hat{T}_R|n\rangle = e^{-i\delta}e^{i\delta}|n\rangle = |n\rangle\,, \tag{C.25}$$

where in the second step we have used the fact that $\hat{T}_R$ is anti-linear, so that $e^{i\delta}$ becomes $e^{-i\delta}$ when you bring it to the left of $\hat{T}_R$. By comparing the left-hand and righ-hand side of the last equality, we clearly see that the assumption that $\hat{T}_R|n\rangle = e^{i\delta}|n\rangle$ is *inconsistent* if $\hat{T}_R^2 = -\mathbb{1}$, and this implies that $\hat{T}_R|n\rangle$ *must be*, in that case, an independent degenerate state with the same energy E_n as $|n\rangle$. Amazing, right?

C.5.1. $\hat{T}_R^2 = \mathbb{1}$: integer spin case.

In the first case, $\hat{T}_R^2 = \mathbb{1}$ and $\hat{K}$ is a unitary and symmetric matrix, $\hat{K}^T = \hat{K}$. Then, a simple proof guarantees that you can always find a unitary matrix $\hat{U}_0$ such that: [8]

$$\hat{K}^T = \hat{K} \qquad \Longrightarrow \qquad \hat{K} = \hat{U}_0\hat{U}_0^T\,. \tag{C.26}$$

Perform now a transformation of the states as $|\psi\rangle \to \hat{U}_0^{-1}|\psi\rangle$, equivalent to a change of basis $|\alpha\rangle \to |\alpha'\rangle = \hat{U}_0|\alpha\rangle$. As you remember, see Eq. C.14, $\hat{K}$ transforms as

$$\hat{K} \to \hat{K}' = \hat{U}_0^{-1}\hat{K}\left(\hat{U}_0^{-1}\right)^T = \mathbb{1}$$

It is a matter of very simple algebra to show that the transformed Hamiltonian, assuming TR-invariance, is symmetric and therefore also *real* (since it is Hermitean):

[8] Any unitary $\hat{K}$ can be expressed as $\hat{K} = e^{i\hat{H}}$ where $\hat{H}$ is Hermitean, as you probably remember from elementary QM. If you don't, diagonalize $\hat{K} = \hat{V}e^{i\hat{\theta}}\hat{V}^\dagger$ through a unitary $\hat{V}$ and the diagonal eigenphases $\hat{\theta}$, and observe that $\hat{H} = \hat{V}\hat{\theta}\hat{V}^\dagger$ is Hermitean and such that $\hat{K} = e^{i\hat{H}}$. Next, it is easy to show that, if $\hat{K}^T = \hat{K}$ then also $\hat{H}^T = \hat{H}$. Take now $\hat{U}_0 = e^{i\hat{H}/2}\hat{O}$ where $\hat{O}$ is any *real orthogonal* operator. Then $\hat{U}_0^T = \hat{O}^T e^{i\hat{H}/2}$ and $\hat{K} = \hat{U}_0\hat{U}_0^T$ because $\hat{O}\hat{O}^T = \mathbb{1}$. As you see, $\hat{U}_0$ is determined up to a real orthogonal transformation $\hat{O}$ which you are free to chose as you wish.

$$\hat{H}' = \hat{U}_0^{-1}\hat{H}\hat{U}_0 = \hat{U}_0^{-1}\left(\hat{K}\hat{H}^T\hat{K}^{-1}\right)\hat{U}_0 = \left(\hat{U}_0^{-1}\hat{H}\hat{U}_0\right)^T = \left(\hat{H}'\right)^T \ . \tag{C.27}$$

This shows the point: if $\hat{T}_R^2 = \mathbb{1}$ (we will see that this correspond to the case when the spin is absent or integer) you can always find a suitable basis in which $\hat{K} = \mathbb{1}$ and the Hamiltonian, being self-dual, is a real symmetric matrix. Notice that at this point you are still free to further change basis with *real orthogonal* transformations $\hat{O}$: the Hamiltonian will still remain real and symmetric for any $\hat{O}$.

C.5.2. $\hat{T}_R^2 = -\mathbb{1}$: half-integer spin case.

This case is definitely quite more complicated. If $\hat{K}$ is unitary and antisymmetric, you cannot find a basis in which it becomes the identity. Still, a theorem guarantees that I can find a unitary transformation which brings $\hat{K}$ into a *canonical form* with blocks on the diagonal made of 2×2 matrices

$$\begin{pmatrix} 0 & +1 \\ -1 & 0 \end{pmatrix} = i\sigma_y \ .$$

So, accept for a second without proof that a unitary $\hat{U}$ exists such that $\hat{K} \to \hat{U}\hat{K}\hat{U}^T = \hat{Z}$ with $\hat{Z}$ given by:

$$\hat{K} \to \hat{U}\hat{K}\hat{U}^T = \hat{Z} \stackrel{def}{=} \begin{bmatrix} 0 & +1 & 0 & 0 & \cdots \\ -1 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & +1 & \cdots \\ 0 & 0 & -1 & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix} \tag{C.28}$$

Notice that if the dimension of the Hilbert space is finite, it must be even for this to make sense: all matrices should be, therefore, $2N \times 2N$. After one such transformation is performed, further unitary transformations $\hat{S}$ should not scramble the nice canonical form of $\hat{Z}$, and for that you must require that:

$$\hat{S}\hat{Z}\hat{S}^T = \hat{Z} \ . \tag{C.29}$$

Notice the difference with the previous $\theta = 0$ case: there the canonical form of $\hat{K}$ was $\hat{K} = \mathbb{1}$ and the group of unitary operators $\hat{O}$ leaving it invariant, i.e., such that $\hat{O}\hat{O}^T = \mathbb{1}$, where simply the real orthogonal transformations, $O(N)$ in the finite-N-dimensional case. Here, the group of unitary $\hat{S}$ which preserves $\hat{Z}$ as in Eq. C.29 is called *symplectic* group, denoted by $Sp(N)$ in the finite-dimensional $2N \times 2N$ case.

How can we justify the fact that a canonical basis of this type must exist? It is enough to think of a Gram-Schmidt orthogonalization process carried on with the help of $\hat{T}_R$. Take a starting state $|\phi_1\rangle$ and form its TR-partner $|\phi_1^R\rangle = \hat{T}_R|\phi_1\rangle$. As proved when we discussed about Kramer's degeneracy, these two states must be linearly independent, indeed orthogonal! Next select one more state $|\phi_2\rangle$, orthogonal to both $|\phi_1\rangle$ and $|\phi_1^R\rangle$, and calculate $|\phi_2^R\rangle$. Again you would prove that the latter is orthogonal to $|\phi_2\rangle$ and to all previously constructed states.

And so on, until you exhaust the Hilbert space. In so doing, you have constructed a complete ortonormal basis made of TR-doublets as follows:

$$\mathcal{H}_{2N} = \{|\phi_1^R\rangle, |\phi_1\rangle, |\phi_2^R\rangle, |\phi_2\rangle, \cdots, |\phi_N^R\rangle, |\phi_N\rangle\} \, . \tag{C.30}$$

In the basis you have just constructed $\hat{T}_R$ coincides with $\hat{K}$ because $\hat{C}$ has no effect on the kets (recall that $\hat{C}$ just takes the complex conjugate of amplitudes in front of kets). Remember also that taking *twice* the time-reversed of a state introduces a minus sign: $\hat{T}_R|\phi_i^R\rangle = -|\phi_i\rangle$. It is then straightforward to conclude that the basis you have constructed is nothing but the *canonical basis* in which $\hat{K}$ has the from in Eq. (C.28). Indeed: $\langle\phi_1^R|\hat{T}_R|\phi_1^R\rangle = 0$, $\langle\phi_1^R|\hat{T}_R|\phi_1\rangle = 1$, $\langle\phi_1|\hat{T}_R|\phi_1^R\rangle = -1$, $\langle\phi_1|\hat{T}_R|\phi_1\rangle = 0$, and so forth.

We stress the fact that the construction of the canonical basis made of TR-doublets is totally *independent* of the fact that $\hat{H}$ is TR-invariant or not: it is enough that $\hat{T}_R^2 = -\mathbb{1}$. But let us know ask: How would the Hamiltonian matrix look in the canonical basis if $\hat{H}$ is TR-invariant? It will look, obviously:

$$[H] = \begin{bmatrix} \begin{pmatrix} \langle\phi_1^R|H|\phi_1^R\rangle & \langle\phi_1^R|H|\phi_1\rangle \\ \langle\phi_1|H|\phi_1^R\rangle & \langle\phi_1|H|\phi_1\rangle \end{pmatrix} & \begin{pmatrix} \langle\phi_1^R|H|\phi_2^R\rangle & \langle\phi_1^R|H|\phi_2\rangle \\ \langle\phi_1|H|\phi_2^R\rangle & \langle\phi_1|H|\phi_2\rangle \end{pmatrix} & \cdots \\ \begin{pmatrix} \langle\phi_2^R|H|\phi_1^R\rangle & \langle\phi_2^R|H|\phi_1\rangle \\ \langle\phi_2|H|\phi_1^R\rangle & \langle\phi_2|H|\phi_1\rangle \end{pmatrix} & \begin{pmatrix} \langle\phi_2^R|H|\phi_2^R\rangle & \langle\phi_2^R|H|\phi_2\rangle \\ \langle\phi_2|H|\phi_2^R\rangle & \langle\phi_2|H|\phi_2\rangle \end{pmatrix} & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix} \tag{C.31}$$

where we have singled-out the 2×2 blocks referring to TR-doublets. Now recall that Eq. (C.22) tells us how operators behave under TR. If I rewrite it for the Hamiltonian it tells us that for any two states $|\phi\rangle$ and $|\psi\rangle$ we have:

$$\langle\phi|\hat{H}|\psi\rangle = \langle\psi^R|\hat{H}^R|\phi^R\rangle \, , \tag{C.32}$$

where $\hat{H}^R = \hat{T}_R\hat{H}^\dagger\hat{T}_R^{-1} = \hat{T}_R\hat{H}\hat{T}_R^{-1}$ is the *dual* of $\hat{H}$ under TR. But if $\hat{H}$ is TR-invariant then $\hat{H}^R = \hat{H}$, which implies that:

$$\langle\phi|\hat{H}|\psi\rangle = \langle\psi^R|\hat{H}|\phi^R\rangle \, . \tag{C.33}$$

The latter is a very strong constraint on the matrix elements of $\hat{H}$ in the canonical basis. Consider for instance the first diagonal block, referring to states $|\phi_1^R\rangle$ and $|\phi_1\rangle$ (all diagonal blocks would do the same). TR-invariance requires that: **1)** $\langle\phi_1^R|H|\phi_1^R\rangle = \langle\phi_1|H|\phi_1\rangle$ (the two minus signs cancel), i.e., the diagonal elements are identical (and real, by Hermiticity); **2)** $\langle\phi_1^R|H|\phi_1\rangle = -\langle\phi_1^R|H|\phi_1\rangle = 0$ (the minus sign originates from the fact that applying TR twice gives a factor -1). Summarizing, we have proved that the diagonal blocks must have the form:

$$\begin{pmatrix} \langle\phi_k^R|H|\phi_k^R\rangle & \langle\phi_k^R|H|\phi_k\rangle \\ \langle\phi_k|H|\phi_k^R\rangle & \langle\phi_k|H|\phi_k\rangle \end{pmatrix} = \begin{pmatrix} u_{kk} & 0 \\ 0 & u_{kk} \end{pmatrix} \, , \tag{C.34}$$

with $u_{kk} \in \mathbb{R}$. Take now an off-diagonal block, for instance the $(2,1)$. Here TR-invariance requires:

$$\begin{pmatrix} \langle\phi_2^R|H|\phi_1^R\rangle & \langle\phi_2^R|H|\phi_1\rangle \\ \langle\phi_2|H|\phi_1^R\rangle & \langle\phi_2|H|\phi_1\rangle \end{pmatrix} = \begin{pmatrix} \langle\phi_1|H|\phi_2\rangle & -\langle\phi_1^R|H|\phi_2\rangle \\ -\langle\phi_1|H|\phi_2^R\rangle & \langle\phi_1^R|H|\phi_2^R\rangle \end{pmatrix} \, , \tag{C.35}$$

and, upon using Hermiticity of the matrix elements, for instance $\langle\phi_1^R|H|\phi_2\rangle = \langle\phi_2|H|\phi_1^R\rangle^*$, you see that this block has the form:

$$\begin{pmatrix} \langle\phi_2^R|H|\phi_1^R\rangle & \langle\phi_2^R|H|\phi_1\rangle \\ \langle\phi_2|H|\phi_1^R\rangle & \langle\phi_2|H|\phi_1\rangle \end{pmatrix} = \begin{pmatrix} u_{21} & -v_{21}^* \\ v_{21} & u_{21}^* \end{pmatrix} . \tag{C.36}$$

An identical conclusion would hold for the block (12):

$$\begin{pmatrix} \langle\phi_1^R|H|\phi_2^R\rangle & \langle\phi_1^R|H|\phi_2\rangle \\ \langle\phi_1|H|\phi_2^R\rangle & \langle\phi_1|H|\phi_2\rangle \end{pmatrix} = \begin{pmatrix} u_{12} & -v_{12}^* \\ v_{12} & u_{12}^* \end{pmatrix} , \tag{C.37}$$

but Hermiticity must relate these factors to the (21) partners. This is best appreciated if we put together these results as follows:

$$[\hat{H}] = \begin{bmatrix} \begin{pmatrix} u_{11} & 0 \\ 0 & u_{11} \end{pmatrix} & \begin{pmatrix} u_{12} & -v_{12}^* \\ v_{12} & u_{12}^* \end{pmatrix} & \cdots \\ \begin{pmatrix} u_{21} & -v_{21}^* \\ v_{21} & u_{21}^* \end{pmatrix} & \begin{pmatrix} u_{22} & 0 \\ 0 & u_{22} \end{pmatrix} & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix} \tag{C.38}$$

Then, you immediately conclude, by Hermiticity, that

$$\begin{aligned} u_{12} &= u_{21}^* \\ v_{12} &= -v_{21} . \end{aligned} \tag{C.39}$$

Hence, we must have:

$$[\hat{H}] = \begin{bmatrix} \begin{pmatrix} u_{11} & 0 \\ 0 & u_{11} \end{pmatrix} & \begin{pmatrix} u_{12} & -v_{12}^* \\ v_{12} & u_{12}^* \end{pmatrix} & \cdots \\ \begin{pmatrix} u_{12}^* & v_{12}^* \\ -v_{12} & u_{12} \end{pmatrix} & \begin{pmatrix} u_{22} & 0 \\ 0 & u_{22} \end{pmatrix} & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix} \tag{C.40}$$

A quite remarkable and bizzare form of $[\hat{H}]$ is forced by TR-invariance in the canonical basis! But to fully understand, appreciate, and work with a matrix having this peculiar form, we have to take a journey into the beautiful world of quaternions.

But before adventuring in that journey, let me mention an alternative way of writing a self-dual Hermitean matrix, as implied by TR-invariance, which was suggested by Valerio Volpati. If you order the basis of TR-states as follows:

$$\mathcal{H}_{2N} = \{|\phi_1^R\rangle, |\phi_2^R\rangle, \cdots |\phi_N^R\rangle, |\phi_1\rangle, |\phi_2\rangle, \cdots, |\phi_N\rangle\} , \tag{C.41}$$

then the matrix $\hat{Z}$ will look, in that basis, as:

$$\hat{Z} = \begin{bmatrix} 0 & \mathbb{1}_N \\ -\mathbb{1}_N & 0 \end{bmatrix} , \tag{C.42}$$

where now $\mathbb{1}_N$ denotes the $N \times N$ unit matrix. You can verify that $\hat{Z}^{-1} = -\hat{Z}$. The requirement that an Hermitean operator is self-dual is, in general, $\hat{H}^R = \hat{T}_R \hat{H} \hat{T}_R^{-1} = \hat{H}$.

In a canonical basis this reads: $\hat{H}^R = \hat{Z}\hat{H}^*\hat{Z}^{-1} = \hat{H}$, where the $*$ denotes the complex conjugation due to the $\hat{C}$, while $\hat{K} = \hat{Z}$. Now if you write the Hamiltonian with four $N \times N$ blocks as follows:

$$\hat{H} = \begin{bmatrix} A & C \\ C^\dagger & B \end{bmatrix} , \tag{C.43}$$

with $A = A^\dagger$ and $B = B^\dagger$, then you immediately see (by carrying out the calculations with the blocks as you would do with 2×2 matrices) that:

$$\hat{H}^R = \hat{Z} \begin{bmatrix} A^* & C^* \\ C^T & B^* \end{bmatrix} \hat{Z}^{-1} = \begin{bmatrix} B^* & -C^T \\ -C^* & A^* \end{bmatrix} . \tag{C.44}$$

Requiring that $\hat{H}^R$ coincides with $\hat{H}$, as implied by TR-invariance, implies that $B = A^*$ and $C = -C^T$ (or, equivalently, $C^\dagger = -C^*$), i.e.,

$$\hat{H} = \begin{bmatrix} A & C \\ -C^* & A^* \end{bmatrix} , \tag{C.45}$$

where $A = A^\dagger$ and $C = -C^T$, i.e, A is Hermitean and C is complex antisymmetric. [9]

C.6. Quaternions

Hamilton was fascinated by the fact that, in the complex plane, a rotation by $\pi/2$ is simply performed through a multiplication by the imaginary unit i, whose square is $i^2 = -1$. [10] He wanted to generalize this construction to represent rotations in three dimensions. To do that, he tried introducing *two* "imaginary units", call them i_1 and i_2, with $i_1^2 = -1$ and $i_2^2 = -1$ and with the associated two imaginary axis. So, in this picture the three-dimensional space would be made of a real axis and two imaginary axis, and the hope would be to get a consistent picture of rotations by identifying vectors (x, y, z) with numbers of the form $x + yi_1 + zi_2$. But that did not work, for a simple reason: While i_1 would rotate x into y, and i_2 would rotate x into z, nothing would rotate y into z. Indeed, if you search for a number w such that $i_2 = wi_1$, you easily conclude (by multiplying things with the given rules) that w cannot be x, a real number, nor of the form xi_1 or xi_2. And you are therefore *forced* to introduce a *third imaginary axis* with its associated "imaginary unit" i_3 such that

$$i_2 = i_3 i_1 .$$

But this immediately implies that multiplication must *not be commutative*, with the given rules. Indeed, by squaring the expression above we get:

$$i_2^2 = -1 = (i_3 i_1)(i_3 i_1) ,$$

[9] Obviously, this structure as well can be described in terms of quaternions, with the only difference that one maps in a rather obvious way the $N \times N$ matrices made of 2×2 blocks into 2×2 matrices made of $N \times N$ blocks.

[10] As you well know, if you identify a vector (x, y) in the Cartesian plane with the complex number $x + iy$, then $i(x + iy) = -y + ix$ represents the vector $(-y, x)$ which is orthogonal to (x, y). Obviously $i^2 = -1$, and this represents a rotation by π.

and you realize that, if multiplication was commutative, the right hand side would be the product of $i_3^2 i_1^2 = (-1)(-1) = +1$, inconsistent with the left hand side! So, together with the rules that $i_1^2 = i_2^2 = i_3^2 = -1$ we must also require that $i_3 i_1 = -i_1 i_3$. Moreover, $i_3 i_2 = i_3(i_3 i_1) = i_3^2 i_1 = -i_1$, and by applying a similar squaring argument as above you must also assume that $i_3 i_2 = -i_2 i_3$, which immediately implies that $i_2 i_3 = i_1$. If you multiply to the left this last expression by i_1 and use that $i_1^2 = -1$ you finally get $i_1 i_2 i_3 = -1$. To summarize, the rules for dealing with these three imaginary units are:

$$\left.\begin{array}{l} i_1^2 = i_2^2 = i_3^2 = -1 \\ i_1 i_2 = -i_2 i_1 = i_3 \\ i_2 i_3 = -i_3 i_2 = i_1 \\ i_3 i_1 = -i_1 i_3 = i_2 \end{array}\right\} \quad \Longrightarrow \quad i_1 i_2 i_3 = -1 \; . \tag{C.46}$$

By definition a *real quaternion* is simply any number of the form:

$$q = x_0 + x_1 i_1 + x_2 i_2 + x_3 i_3 \qquad \text{with } \; x_0, x_1, x_2, x_3 \in \mathbb{R} \; , \tag{C.47}$$

and can be clearly identified with a point $(x_0, x_1, x_2, x_3) \in \mathbb{R}^4$. To efficiently perform calculations, it is usueful to use a more compact notation, like, $q = x_0 + \sum_{n=1}^{3} x_n i_n$, or simply $q = x_0 + \sum_n x_n i_n$. Moreover, the rules given above should remind you of vector-product rules. Indeed, by introducing the totally antisymmetric tensor $\epsilon^{lmn} = \pm 1$ which you are likely familiar with in vector calculus, you can convince youself that the rules for multiplying the imaginary units nicely sum-up into: [11]

$$i_l i_m = \epsilon^{lmn} i_n - \delta_{lm} \; . \tag{C.48}$$

A very useful quantity is the *conjugate* $\overline{q}$ of a quaternion q, defined as:

$$\overline{q} = x_0 - \sum_{n=1}^{3} x_n i_n \; . \tag{C.49}$$

By using the rules in Eq. (C.48) it takes very little to show that

$$q\overline{q} = x_0^2 + \sum_{n=1}^{3} x_n^2 \overset{def}{=} |q|^2 \; , \tag{C.50}$$

where we have defined the squared-norm of q in the standard Euclidean way. Notice that $|q|^2 = 0$ only if $q = 0$. But you should be careful with the conjugation: conjugation of a product exchanges the order, as you are accostumed to with matrices [12]

$$\overline{q_1 q_2} = \overline{q_2}\;\overline{q_1} \; . \tag{C.51}$$

[11] Imagine you have two three-dimensional vectors $\mathbf{x}$ and $\mathbf{y}$ and you define the associated quanternions $q_{\mathbf{x}} = \sum_n x_n i_n$ and $q_{\mathbf{y}} = \sum_n y_n i_n$ (notice that both $x_0 = y_0 = 0$). Then, you easily conclude that

$$q_{\mathbf{x}} q_{\mathbf{y}} = -(\mathbf{x}\cdot\mathbf{y}) + \sum_n (\mathbf{x}\times\mathbf{y})_n i_n \; ,$$

i.e., quaternion products contain both scalar and vector product components.

[12] A simple consequence of these definitions and properties is that

$$|q_1 q_2|^2 = q_1 q_2 \overline{q_1 q_2} = q_1 q_2 \overline{q_2}\;\overline{q_1} = |q_1|^2 |q_2|^2 \; .$$

Therefore $q_1 q_2 = 0$ implies that either $q_1 = 0$ or $q_2 = 0$, which allows to introduce the operation of *division*. With divisions at hand, you might define derivatives and, in principle, one could develop a whole *quaternion calculus*: we will not enter into that.

So far we have dealt with *real quaternions*, but you realize that one can introduce also *complex quaternions*, or *bi-quaternions*

$$q = z_0 + \sum_{n=1}^{3} z_n i_n \quad \text{with } z_0, z_1, z_2, z_3 \in \mathbb{C} \,, \tag{C.52}$$

which can be identified with a point $(z_0, z_1, z_2, z_3) \in \mathbb{C}^4$. [13] For complex quaternions you can define not only the conjugate $\overline{q}$ but also the "complex conjugate" q^* as:

$$q^* \stackrel{def}{=} z_0^* + \sum_{n=1}^{3} z_n^* i_n \,, \tag{C.53}$$

and the Hermitean conjugate

$$q^\dagger \stackrel{def}{=} \overline{q}^* = z_0^* - \sum_{n=1}^{3} z_n^* i_n \,. \tag{C.54}$$

A quaternion is *Hermitean* if $q^\dagger = q$, which requires, as you can easily show, that $z_0 = x_0 \in \mathbb{R}$ and $z_n = i x_n$ with $x_n \in \mathbb{R}$. [14]

The reason for introducing quaternions (apart from their intellectual beauty) is that they are *deeply related to Pauli matrices* and spin-1/2 operators. Let us see why. You certainly remember that Pauli matrices σ_1, σ_2, σ_3 verify the following relationships:

$$\begin{aligned} &\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = \mathbb{1} \\ &\sigma_1\sigma_2 = -\sigma_2\sigma_1 = i\sigma_3 \\ &\sigma_2\sigma_3 = -\sigma_3\sigma_2 = i\sigma_1 \\ &\sigma_3\sigma_1 = -\sigma_1\sigma_3 = i\sigma_2 \end{aligned} \tag{C.55}$$

You therefore realize that you can get a *representation of quaternion algebra* with the following Pauli-matrix identification:

$$\begin{aligned} i_1 &\rightarrow i\sigma_3 = \begin{pmatrix} +i & 0 \\ 0 & -i \end{pmatrix} \\ i_2 &\rightarrow i\sigma_2 = \begin{pmatrix} 0 & +1 \\ -1 & 0 \end{pmatrix} \\ i_3 &\rightarrow i\sigma_1 = \begin{pmatrix} 0 & +i \\ +i & 0 \end{pmatrix} \end{aligned} \tag{C.56}$$

where you should remember the extra i and the exchange of the indices 1 and 3. If you further identify 1 with the 2×2 identity matrix $\mathbb{1}$ you can come up with a representation of a *real* quaternion $q = x_0 + \sum_n x_n i_n$ in terms of the following 2×2 matrix

$$q = x_0 + \sum_n x_n i_n = \begin{pmatrix} x_0 + ix_1 & x_2 + ix_3 \\ -x_2 + ix_3 & x_0 - ix_1 \end{pmatrix} = \begin{pmatrix} u & -v^* \\ v & u^* \end{pmatrix} \,, \tag{C.57}$$

[13] It is important not to mix the imaginary unit i of complex numbers with the quaternions i_1, i_2, i_3: they have nothing to do with each other, although they share the fact that their square is -1.

[14] These Hermitean quaternions are particularly usuful in special relativity.

with $u = x_0 + ix_1$ and $v = -x_2 + ix_3$. This apparently unusual form is what Time Reversal invariance implies when there are spin-1/2 around, see Sec. C.5.2.

But before ending this journey into the quaternion world, let us notice that if you consider an *Hermitean quanternion* $q = x_0 + \sum_n (ix_n) i_n = q^\dagger$, then the 2×2 matrix representing it is an Hermitean matrix:

$$q = x_0 + \sum_n (ix_n) i_n = \begin{pmatrix} x_0 - x_1 & ix_2 - x_3 \\ -ix_2 - x_3 & x_0 + x_1 \end{pmatrix} . \tag{C.58}$$

Let me stress that the representations of the quaternions in terms of 2×2 matrices given in Eq. (C.56) is not the only one possible: it is the one used by Metha, and that is the reason I have used it here. [15] With this choice of representation, Hermitean matrices appear a bit clumsy. A better choice to make them look nicer would be:

$$\begin{aligned} i_1 \quad &\to \quad -i\sigma_1 = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} \\ i_2 \quad &\to \quad -i\sigma_2 = \begin{pmatrix} 0 & -1 \\ +1 & 0 \end{pmatrix} \\ i_3 \quad &\to \quad -i\sigma_3 = \begin{pmatrix} -i & 0 \\ 0 & +i \end{pmatrix} \end{aligned} \tag{C.59}$$

in terms of which an Hermitean quaternion $q = x_0 + \sum_n (ix_n) i_n$ reads:

$$q = x_0 + \sum_n (ix_n) i_n = \begin{pmatrix} x_0 + x_3 & x_1 - ix_2 \\ x_1 + ix_2 & x_0 - x_3 \end{pmatrix} = x_0 \mathbb{1} + \mathbf{x} \cdot \boldsymbol{\sigma} . \tag{C.60}$$

C.7. Quaternions, TR-invariance, and Symplectic group for half-integer spin case

Now that we know quaternions, let us go back to the form that TR-invariance requires for the Hamiltonian matrix when $\hat{T}_R^2 = -\mathbb{1}$. We can now write every 2×2 block appearing in $[\hat{H}]$ in Eq. (C.38) as a quaternion, in the form: [16]

$$[\hat{H}] = [Q] = \begin{bmatrix} q_{11} & q_{12} & q_{13} & \cdots & q_{1N} \\ q_{21} & q_{22} & q_{23} & \cdots & q_{2N} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ q_{N1} & q_{N2} & q_{N3} & \cdots & q_{NN} \end{bmatrix} \tag{C.61}$$

As we have seen, all these are *real quaternions* (see Eqs. (C.36) and (C.57)), which obviously does not mean that the matrix is real! [17] If we write every quaternion in the standard way

[15] Metha denotes the quaternions by e_1, e_2 and e_3 rather than with i_1, i_2 and i_3.

[16] Notice that the ordinary rules of matrix multiplications are not changed by the 2×2 partitioning.

[17] We might also show, following Metha, that standard matrix operations are reflected in $[Q]$ as follows:

$$[Q^T]_{kl} = -i_2 \overline{q}_{lk} i_2 \qquad [Q^\dagger]_{kl} = q^\dagger_{lk} \qquad [Q^R]_{kl} = i_2 [Q^T]_{kl} i_2^{-1} = \overline{q}_{lk} . \tag{C.62}$$

It follows that a quaternion matrix $[Q]$ such that $[Q^\dagger] = [Q^R]$ is *quaternion real*.

(just shift up the quaternion indices $0, \cdots, 3$ to make space for the new matrix indices) as:

$$q_{kl} = x^{(0)}_{kl} + x^{(1)}_{kl} i_1 + x^{(2)}_{kl} i_2 + x^{(3)}_{kl} i_3 = \begin{pmatrix} \underbrace{x^{(0)}_{kl} + i x^{(1)}_{kl}}_{u_{kl}} & \underbrace{x^{(2)}_{kl} + i x^{(3)}_{kl}}_{-v^*_{kl}} \\ \underbrace{-x^{(2)}_{kl} + i x^{(3)}_{kl}}_{v_{kl}} & \underbrace{x^{(0)}_{kl} - i x^{(1)}_{kl}}_{u^*_{kl}} \end{pmatrix} , \tag{C.63}$$

then we see immediately that along the main diagonal we must have:

$$q_{kk} = x^{(0)}_{kk} = \overline{q}_{kk} \, . \tag{C.64}$$

Moreover, see Eq. (C.39), Hermiticity requires that $q_{12} = \overline{q}_{21}$, etc. In summary, the real-quaternion matrix $[Q]$ representing $\hat{H}$ in the canonical basis has real quaternion elements which satisfy: [18]

$$q_{lk} = \overline{q}_{kl} \, . \tag{C.65}$$

In terms of quaternions, we can write the canonical form of the unitary component $\hat{K}$ of TR using i_2 as:

$$[\hat{K}] = [\hat{Z}] = \begin{bmatrix} i_2 & 0 & 0 & \cdots & 0 \\ 0 & i_2 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & i_2 \end{bmatrix} = i_2 [\mathbb{1}] \, . \tag{C.66}$$

Finally, further change of basis from the canonical basis we have selected are possible as long as the new basis is canonical as well, i.e., in it $[\hat{K}] = [\hat{Z}] = i_2[\mathbb{1}]$. As we have mentioned, the unitary transformations $\hat{S}$ that conserve this canonical form are a group, the *symplectic group*:

$$\hat{S} \hat{Z} \hat{S}^T = \hat{Z} \, . \tag{C.67}$$

If you calculate $\hat{S}^R = \hat{Z} \hat{S}^T \hat{Z}^{-1}$ (this is what the R of an operator/matrix is defined to be) you immediately see that a sympletic transformation is such that $\hat{S}^R = \hat{S}^{-1}$. But they are also unitary, so:

$$\hat{S}^R = \hat{S}^{-1} = \hat{S}^\dagger \, . \tag{C.68}$$

Written in terms of quaternions, symplectic transformations can be shown to be *quaternion real* as well (but not Hermitean).

So, summarizing, TR-invariance when $\hat{T}_R^2 = -\mathbb{1}$ implies that the Hamiltonian is quaternion real and self-dual, $q_{kl} = \overline{q}_{lk}$, and you can still make a change of canonical basis by symplectic unitary transformations, which are also represented by quaternion real matrices.

C.7.1. A simple illustration: Spin-orbit coupling in the p states of hydrogen

After this rather long formal trip, let us take a break and illustrate some of the results we have found in simple terms. The exercise I propose is studying the form of the spin-orbit coupling term $\lambda(r) \mathbf{L} \cdot \mathbf{S}$, evidently a TR-invariant term, within the restricted subpsace of a given multiplet of p orbitals of hydrogen: as you probably know, this is one of the ingredients

[18] If we construct $N \times N$ real matrices $\mathbf{x}^{(0)}$, $\mathbf{x}^{(1)}$, $\mathbf{x}^{(2)}$, and $\mathbf{x}^{(3)}$ then we see that $q_{lk} = \overline{q}_{kl}$ implies that $\mathbf{x}^{(0)}$ is symmetric, while $\mathbf{x}^{(1,2,3)}$ are antisymmetric.

(in a perturbative approach, justified by the smallness of the fine-structure constant α) of the *fine-structure* of the resulting levels. Ideally, you should try to do the calculations yourself, without looking at the answer, in a kind of guided exercise.

So, we consider the p states, whose angular wave-function is given by the spherical harmonics $Y_{1,m}(\theta,\phi)$. If you open-up a book in Quantum Mechanics, you will find that they read:

$$\begin{array}{lll} Y_{1,+1} & = -e^{i\delta}\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi} & = -e^{2i\delta}Y^*_{1,-1} \\ Y_{1,0} & = e^{i\delta}\sqrt{\frac{3}{4\pi}}\cos\theta & = e^{2i\delta}Y^*_{1,0} \\ Y_{1,-1} & = e^{i\delta}\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{-i\phi} & = -e^{2i\delta}Y^*_{1,+1} \end{array} \quad . \tag{C.69}$$

To be honest, in essentially any book you would find these expressions but with a choice of phase $\delta = 0$. The reason I have included this extra phase is just to show that it is largely *arbitrary* but, as you will see, *infinitely irrelevant*. Notice also the minus sign difference between $Y_{1,+1}$ and $Y_{1,-1}$, which is due to the effect of L^-. So, summarizing, complex conjugation $\hat{C}$ changes $m \to -m$ apart from some phase factors which, in any case, disappear if we apply $\hat{C}^2$.

Now consider the spin-1/2 states of the electron. We will use the standard basis of S^z, $|\uparrow\rangle$ and $|\downarrow\rangle$. Any spin-wavefunction with *real coefficients* (a state in the xz plane in spin space) will not be affected by $\hat{C}$, while, for instance, for the eigenstates of S^y:

$$\begin{array}{l} |+\rangle_y = \frac{1}{\sqrt{2}}(|\uparrow\rangle + i|\downarrow\rangle) = \hat{C}|-\rangle_y \\ |-\rangle_y = \frac{1}{\sqrt{2}}(|\uparrow\rangle - i|\downarrow\rangle) = \hat{C}|+\rangle_y \end{array} \tag{C.70}$$

$\hat{C}$ is enough to reverse the spin. Evidently, to reverse the spin in any direction we need an operator which turns the spin around y by π, so as to reverse the xz spins. This operator should be:

$$\hat{T}_R = \hat{K}\hat{C} = e^{i\pi S^y/\hbar}\hat{C} = e^{i\frac{\pi}{2}\sigma^y}\hat{C} = i\sigma^y\hat{C}\ , \tag{C.71}$$

where $\hat{C}$ takes care of reversing momenta, orbital angular momenta, and spin-components along y, while $\hat{K} = e^{i\frac{\pi}{2}\sigma^y} = i\sigma_y$ has no effect on spin-components along y, but reverses spin-components in the xz plane (unaffected by $\hat{C}$). With this choice:

$$\begin{array}{ll} \hat{T}_R|\uparrow\rangle & = -|\downarrow\rangle \\ \hat{T}_R|\downarrow\rangle & = +|\uparrow\rangle \end{array} \quad . \tag{C.72}$$

Notice the minus sign: we will see it is the crucial minus sign in this story. With the $Y_{1,m}$ as defined above, you immediately derive:

$$\begin{array}{ll} \hat{T}_R Y_{1,+1}|\uparrow\rangle & = +e^{-2i\delta}Y_{1,-1}|\downarrow\rangle \\ \hat{T}_R Y_{1,-1}|\downarrow\rangle & = -e^{-2i\delta}Y_{1,+1}|\uparrow\rangle \\ \hline \hat{T}_R Y_{1,0}|\uparrow\rangle & = -e^{-2i\delta}Y_{1,0}|\downarrow\rangle \\ \hat{T}_R Y_{1,0}|\downarrow\rangle & = +e^{-2i\delta}Y_{1,0}|\uparrow\rangle \\ \hline \hat{T}_R Y_{1,-1}|\uparrow\rangle & = +e^{-2i\delta}Y_{1,+1}|\downarrow\rangle \\ \hat{T}_R Y_{1,+1}|\downarrow\rangle & = -e^{-2i\delta}Y_{1,-1}|\uparrow\rangle \end{array} \tag{C.73}$$

To stress the fact that $\hat{T}_R$ couples states *in pairs*, I have put horizontal lines between the 3 TR doublets that we have. With these choices, the matrix representing $\hat{T}_R$ in this basis will

have 2×2 blocks along the main diagonal of the form:

$$\begin{pmatrix} 0 & \pm e^{-2i\delta} \\ \mp e^{-2i\delta} & 0 \end{pmatrix} . \tag{C.74}$$

It is now clear that, depending on: 1) the *ordering* of the states $|\phi_i\rangle$ and $|\phi_i^R\rangle$, and 2) the *phase* you absorb in their definition, you can make most of the phases to disappear and reduce to blocks of the canonical form:

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} . \tag{C.75}$$

For instance, take:

$$\{|\phi_1^R\rangle = e^{-i\delta}|1,-1\rangle|\downarrow\rangle \; ; |\phi_1\rangle = e^{-i\delta}|1,+1\rangle|\uparrow\rangle\} \tag{C.76}$$

and the resulting block will be canonical. Similarly, take:

$$\{|\phi_2^R\rangle = -e^{-i\delta}|1,0\rangle|\downarrow\rangle \; ; |\phi_2\rangle = e^{-i\delta}|1,0\rangle|\uparrow\rangle\} \tag{C.77}$$

and the corresponding block will be also canonical. And so on.

You still might wonder: where does the important minus sign in $\hat{T}_R^2 = -\mathbb{1}$ comes from, in the end? From the spin-1/2 algebra! Indeed, you immediately see that:

$$\hat{T}_R^2 = e^{i\frac{\pi}{2}\sigma^y}\hat{C}e^{i\frac{\pi}{2}\sigma^y}\hat{C} = e^{i\frac{\pi}{2}\sigma^y}\left(e^{i\frac{\pi}{2}\sigma^y}\right)^* = e^{i\frac{\pi}{2}\sigma^y}e^{i\frac{\pi}{2}\sigma^y} = e^{i\pi\sigma^y} = -1 \tag{C.78}$$

C.7.2. Integer versus half-integer spins

If I have N spin-1/2 particles, then:

$$\hat{T}_R = e^{i\pi\mathbf{S}_1^y/\hbar}e^{i\pi\mathbf{S}_2^y/\hbar}\cdots e^{i\pi\mathbf{S}_N^y/\hbar}\hat{C} \, , \tag{C.79}$$

Then it is clear the $\hat{T}_R^2 = (-1)^N\mathbb{1}$. The case of integer spin can be regarded as the N-even case of the previous formula. Integer spins, therefore, have $\hat{T}_R^2 = \mathbb{1}$.

C.8. Time-reversal invariance for time-dependent Hamiltonians.

Let us consider again the general case in which $\hat{H}(t)$ is time-dependent. Assume that there is a time t_0 around which there is TR-invariance. As previously discussed (see Eqs. (C.7) and (C.8)) this implies that:

$$\begin{aligned} \hat{U}(t,t_0)\hat{T}_R &= \hat{T}_R\hat{U}(2t_0-t,t_0) \\ \hat{H}(t)\hat{U}(t,t_0)\hat{T}_R &= \hat{T}_R\hat{H}(2t_0-t)\hat{U}(2t_0-t,t_0) \, . \end{aligned} \tag{C.80}$$

Substituting the first condition in the second one, we immediately deduce, getting rid of a factor $\hat{U}(2t_0-t,t_0)$, that:

$$\hat{T}_R^{-1}\hat{H}(t)\hat{T}_R = \hat{H}(2t_0-t) \qquad \Longleftrightarrow \qquad \text{TR-invariance holds} \, . \tag{C.81}$$

Notice that this implies that, generally, $\hat{H}(t)$ does *not commute* with $\hat{T}_R$, except at the "center-of-symmetry" special time t_0:

$$\hat{T}_R^{-1}\hat{H}(t_0)\hat{T}_R = \hat{H}(t_0) \ .$$

Very special is, in that respect, the case of a *time-periodic* $\hat{H}(t)$, i.e., when a period τ exists such that $\hat{H}(t+\tau) = \hat{H}(t)$. Then, if t_0 is the center of TR-symmetry, consider what happens at $t = t_0 \pm \tau/2$. We have:

$$\hat{T}_R^{-1}\hat{H}(t_0 \pm \frac{\tau}{2})\hat{T}_R = \hat{H}(2t_0 - (t_0 \pm \frac{\tau}{2})) = \hat{H}(t_0 \mp \frac{\tau}{2}) = \hat{H}(t_0 \pm \frac{\tau}{2}) \ ,$$

where the last equality follows from the τ-periodicity of $\hat{H}(t)$. Hence, we have proved that $\hat{H}(t)$ commutes with $\hat{T}_R$ not only at t_0, but also at $t = t_0 \pm \tau/2$, and (as you can easily show) at all the other period-related times.

The periodic case is indeed quite surprising in many respects. Suppose you have:

$$\hat{H}(t) = \hat{H}_0 + \hat{V}\sin(\omega_0 t) \ .$$

Assume that $\hat{T}_R^{-1}\hat{H}_0\hat{T}_R = \hat{H}_0$, and that $\hat{V}$ is *odd* under TR, i.e., $\hat{T}_R^{-1}\hat{V}\hat{T}_R = -\hat{V}$. The TR-invariance is actually respected by the dynamics, since, according to Eq. (C.81) (with $t_0 = 0$):

$$\hat{T}_R^{-1}\hat{H}(t)\hat{T}_R = \hat{H}(-t) \ . \tag{C.82}$$

So, a magnetic field term (odd under TR) might be present and still TR holds! You might think that this happens only because we have used the $\sin(\omega_0 t)$, which is odd under $t \to -t$, but indeed the result is more general! You can verify that TR is obeyed even when you use $\cos(\omega_0 t)$, provided this time you use $2t_0 = \pi/\omega_0$ as "center-of-symmetry" for TR. Moreover, you can have a $\hat{V}$ that is *even* under TR, multiplied by $\sin(\omega_0 t)$ and still keep TR-invariance, but again with $2t_0 = \pi/\omega_0$. In general you can prove that TR holds, for a judicious choice of t_0, for any $\hat{H}(t)$ of the form:

$$\hat{H}(t) = \hat{H}_0 + \hat{V}\cos(\omega_0 t + \varphi_0) \ ,$$

as long as $\hat{H}_0$ is TR-invariant, and $\hat{V}$ is either *even* or *odd* under TR.

Another consequence of TR for time-periodic systems is the following. Suppose that TR holds with $t_0 = 0$. Then:

$$\hat{U}(\tau, 0)\hat{T}_R = \hat{T}_R\hat{U}(-\tau, 0) \ .$$

But Floquet theorem guarantees (see Chapter on Floquet systems) that $\hat{U}(-\tau, 0) = \hat{U}(0, \tau)$. On the other hand, quite generally you have that $\hat{U}(0, \tau) = \hat{U}^{-1}(\tau, 0) = \hat{U}^\dagger(\tau, 0)$. Hence, we conclude that:

$$\hat{U}(\tau, 0)\hat{T}_R = \hat{T}_R\hat{U}^\dagger(\tau, 0) \quad \Longrightarrow \quad \hat{U}(\tau, 0) = \hat{T}_R\hat{U}^\dagger(\tau, 0)\hat{T}_R^{-1} \ .$$

And here we should distinguish if the system has spin or not. The easy case is when $\hat{T}_R = \hat{C}$, up to a unitary transformation $\hat{K}$. Then the last equation implies that:

$$\hat{U}(\tau, 0) = \hat{T}_R\hat{U}^\dagger(\tau, 0)\hat{T}_R^{-1} = \hat{U}^T(\tau, 0) \ ,$$

i.e., we can always find a basis in which the Floquet evolution operator over one period coincides with its *transpose*, hence is *unitary and symmetric*. If there are half-integer spin, then you should work a bit more. Try.

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