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Non-equilibrium quantum systems

(Updated lecture-notes)

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Preface

This is a continuously updated version of the lecture notes for the Course on "Non-equilibrium quantum systems" held within the Spring College on "Physics of Complex Systems". Please check the College website regularly for updates.

Contents

1. Thouless adiabatic pump: generalities

We plan to investigate here a very instructive example, the Thouless adiabatic pump [1], which shows many ingredients at play: non-equilibrium physics (in the adiabatic regime), with non-trivial topological properties as a manifestation of Berry phase in transport. Apart from being very instructive, the interest in this problem has been revived recently by the appearence of two different experiments, exploiting cold atoms settings, where the idea is explicitly realized and demonstrated. In one experiment [2], from the group of I. Bloch, they use ^{87}Rb (bosonic) atoms; in the other [3], ^{171}Yb (fermionic) atoms, with two hyperfine nuclear levels playing the role of the fermionic spin 1/2. The interested reader can also profit from the reading of Raffaele Resta's lecture notes [4, Sec. 4.6 and Chap. 5], where the connection with the modern theory of electronic polarization is explained in detail.

1.1. Setting up the problem on the continuum

The problem that Thouless concieved is that of an insulator (in one dimension) which is subject to a time-dependent potential term which tends to drive the system in one direction. You could write the Hamiltonian as:

$$\widehat{H}(t) = \sum_{j=1}^{N} \left(\frac{\hat{p}_j^2}{2m} + V_s(x_j) + V_l(x_j - vt) \right) + \frac{1}{2} \sum_{i \neq j} V_{\text{int}}(|x_i - x_j|) \, . \tag{1.1}$$

In the recent experimental realizations

$$V_s(x) = V_s \sin^2 \left(\frac{\pi x}{d_s} + \frac{\pi}{2} \right)$$

is a standing wave sinusoidal potential induced by a pair of counter-propagating lasers with a certain wavelength, resulting in periodic potential with period d_s. V_l is a similar potential with a longer periodicity d_l, such that $d_s = \alpha d_l$ and $\alpha = 1/2$:

$$V_l(x - vt) = V_l \sin^2 \left(\frac{\pi(x - vt)}{d_l} \right) = V_l \sin^2 \left(\frac{\pi x}{d_l} - \frac{\varphi(t)}{2} \right)$$

where $\varphi(t) = 2\pi t/T = 2\pi vt/d_l$. As you see, the Hamiltonian is time-periodic, i.e., $\widehat{H}(t = T) = \widehat{H}(t = 0)$ in such a setting. Moreover, for any fixed t, the potential is periodic with a lattice constant $a = d_l = 2d_s$ for the present choice of α. Fig. 1.1 shows this potential for several values of the phase difference φ.

The assumption that Thouless made is that the system is an *insulator*, i.e., if $\widehat{J}_x$ denotes the total current operator in the x-direction, and $|\Psi(0)\rangle$ is the ground state of $\widehat{H}(0)$, then

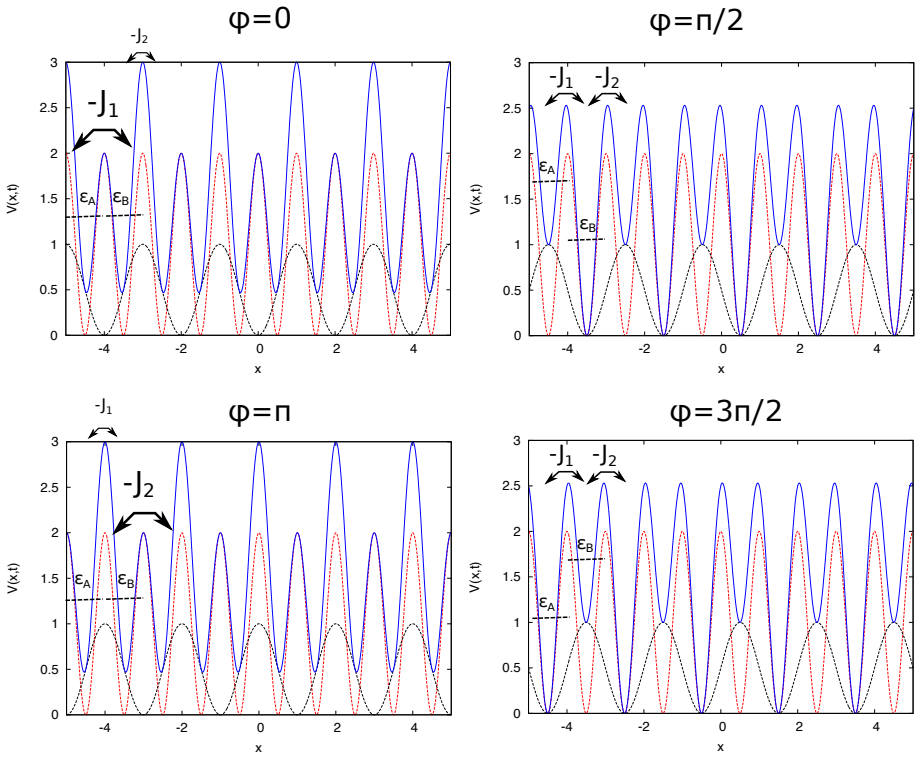

Figure 1.1.: The potential used in the experimental realization of the Thouless pump at different values of the phase difference φ. The tight-binding parameters used in the Rice-Mele model, indicated in the figure, will be explained later on.

$\langle\Psi(0)|\widehat{J}_x|\Psi(0)\rangle = 0$. [1] But the surprising feature that Thouless pointed out is that even insulators, in some cases, can transport charge. In particular, you can calculate the charge transported in a period T as:

$$Q = \lim_{L\to\infty} \frac{1}{L} \int_0^T dt\, \langle\Psi(t)|\widehat{J}_x|\Psi(t)\rangle \,, \tag{1.2}$$

and you will find that, provided the adiabatic condition holds — i.e., T is long enough —, this Q can be different from 0 in some cases, although necessarily an *integer*. In other words the adiabatically pumped charge is necessarily quantized. The cases where $Q \neq 0$ are associated to non-trivial topological features of the insulator.

In order to proceed in this journey, we have to learn a few basic things, starting from the form of the current operator, and continuing with learning the rules-of-the-game of the adiabatic theorem and Berry phase. Let us consider these ingredients one after the other.

1.2. The current and the trick of twisted boundary conditions

You have encountered the current in elementary quantum mechanics. You remember that, for a single particle in, say, one dimension, the current density (omitting the charge $-e$ in

[1] For an insulator, the current would identically vanish even in presence of a small force which tends to drift the particles: a small electric field, if the particles are charged.

front, if you are dealing with, say, electrons) would be given by

$$j(x) = \frac{1}{2m}\Big(\psi^*(x)[\hat{p}\psi(x)] + [\hat{p}\psi(x)]^*\psi(x)\Big) .$$

It is essentially the sandwitch of the momentum operator $\hat{p} = -i\hbar\partial_x$, which can however be applied either to the ket to the right, or to the bra on the left, in a completely symmetric fashion (in such a way that the result is real, i.e., the second term is the complex conjugate of the first). If you integrate over all x, you get the total current as

$$J = \int_{-\infty}^{\infty} dx\; j(x) = \frac{1}{2m}\Big(\langle\psi|\hat{p}\psi\rangle + \langle\hat{p}\psi|\psi\rangle\Big) = \langle\psi|\frac{\hat{p}}{m}|\psi\rangle ,$$

i.e., essentially, the velocity. Hence, you can say that the total current *operator* is $\widehat{J} = \hat{p}/m$. All this should be known and rather elementary. Now I tell you a useful trick that allows to calculated the average total current in a very handy way, a trick invented by Kohn long ago, and which has to do with working with boundary conditions. Consider, to start with, a free particle, say in two-dimensions. Its Hamiltonian is:

$$\widehat{H} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} .$$

The particle stays in a finite rectangular region $L_x \times L_y$, but to solve the problem I have to specify the boundary conditions used. A standard assumption is that periodic boundary conditions (PBC) are used, i.e., the solutions of $\widehat{H}\psi(x,y) = E\psi(x,y)$ should be such that $\psi(x+L_x,y) = \psi(x,y)$ and $\psi(x,y+L_y) = \psi(x,y)$. Physically, if L_x is large enough [2] you can picture the x-PBC as having the particle on a cylinder of circumpherence L_x, while the y-PBC would be picture as closing the cylinder into a torus. But let us forget about y-PBC and leave the cylinder open. You can think of inserting at the center of the cylinder a magnetic fluex Φ, which will induce a constant vector potential A_Φ directed along the circumpherence of the cylinder, $A_\Phi = \Phi/L_x$ by Stokes theorem. Hence the Hamiltonain on the cylinder in the presence of the flux would read

$$\widehat{H}(\Phi) = \frac{\left(\hat{p}_x + \frac{e\Phi}{cL_x}\right)^2}{2m} + \frac{\hat{p}_y^2}{2m} .$$

Question: can we get rid of this constant vector potential term from the Hamiltonian? Answer: Yes, but the wavefunction would no longer be obeying PBC! Indeed, let us define new wavefunctions given by

$$\widetilde{\psi}_\kappa(x,y) = \mathrm{e}^{i\kappa x}\psi(x,y) .$$

The transformation has to be implemented on the Hamiltonian as well, by the unitary transformation $\widetilde{H}_\kappa = \mathrm{e}^{i\kappa x}\widehat{H}(\Phi)\mathrm{e}^{-i\kappa x}$. A simple calculation shows that $\mathrm{e}^{i\kappa x}\hat{p}_x\mathrm{e}^{-i\kappa x} = \hat{p}_x - \hbar\kappa$. Hence, the transformed Hamiltonian is

$$\widetilde{H}_\kappa = \frac{\left(\hat{p}_x + \frac{e\Phi}{cL_x} - \hbar\kappa\right)^2}{2m} + \frac{\hat{p}_y^2}{2m} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} ,$$

where the last equality follows for the obviously optimal choice

$$\hbar\kappa = \frac{e\Phi}{cL_x} \qquad \Longrightarrow \qquad \kappa = \frac{2\pi}{L_x}\frac{\Phi}{\Phi_0} , \tag{1.3}$$

[2] A cylinder has a curvature, but if L_x is large enough, it does not matter.

where $\Phi_0 = hc/e$ is the *flux quantum*. The transformed wave-funcions $\widetilde{\psi}_\kappa(x,y)$ carry the information of the flux by obeying *twisted* boundary conditions:

$$\widetilde{\psi}_\kappa(x+L_x,y) = \mathrm{e}^{i\kappa L_x}\widetilde{\psi}_\kappa(x,y)\ . \tag{1.4}$$

All this is very general, and applies to many particles, even in presence of external potential and interactions. For instance, the Hamiltonian in the presence of a flux, for the one-dimensional problem we are dealing with (on the cylinder), would be:

$$\widehat{H}(\kappa,t) = \sum_{j=1}^{N}\Big(\frac{(\hat{p}_j+\hbar\kappa)^2}{2m} + V_s(x_j) + V_l(x_j-vt)\Big) + \frac{1}{2}\sum_{i\neq j} V_{\rm int}(|x_i-x_j|)\ . \tag{1.5}$$

As explained above, it would be totally equivalent to solve the same problem with κ not appearing in the Hamiltonian, but appearing in the wave-funcions as a twist of the boundary condition for each particle: $\widetilde{\psi}_\kappa(\cdots,x_j+L_x,\cdots) = \mathrm{e}^{i\kappa L_x}\widetilde{\psi}_\kappa(\cdots,x_j,\cdots)$. But even more important to us is the fact that you can easily write down the total current operator as

$$\widehat{J} = \frac{1}{\hbar}\frac{\partial\widehat{H}(\kappa,t)}{\partial\kappa}\Big|_{\kappa=0} = \sum_j \frac{\hat{p}_j}{m}\ , \tag{1.6}$$

whose usefulness will become clear in a moment.

Before ending this section, let us observe the strong similarity between this result and a well known fact about Bloch wavefunctions in crystalline systems. You know that, in band theory, you can classify the single-particle states of a particle moving in a periodic potential $v(x+a)=v(x)$ (for simplicity, we treat the one-dimensional case) through Bloch waves of the form

$$\psi_{nk}(x) = \mathrm{e}^{ikx}u_{nk}(x) \tag{1.7}$$

where $u_{nk}(x) = u_{nk}(x+a)$ is a periodic function, k is a wave-vector which you can take to be in the first Brillouin zone (BZ) of the reciprocal lattice $k\in(-\pi/a,\pi/a]$, and n the so-called band-index. The band dispersion ϵ_{nk} is nothing but the eigenvalue in $\widehat{H}\psi_{nk}=\epsilon_{nk}\psi_{nk}$, with $\widehat{H}=\hat{p}^2/(2m)+v(x)$. You can ask yourself what is the (time-independent) Schrödinger equation that the u_{nk} satisfy. You realize that you have to do essentially the same algebra as above: $u_{nk}(x)$ satisfies:

$$\underbrace{\mathrm{e}^{-ikx}\widehat{H}\mathrm{e}^{ikx}}_{\widehat{H}(k)}\,u_{nk}(x) = \epsilon_{nk}\,u_{nk}(x)\ ,$$

and the Hamiltonian $\widehat{H}(k)$ is given by

$$\widehat{H}(k) = \mathrm{e}^{-ikx}\widehat{H}\mathrm{e}^{ikx} = \frac{(\hat{p}+\hbar k)^2}{2m} + v(x)\ .$$

The advantage of working with $u_{nk}(x)$, rather than with $\psi_{nk}(x)$, is that all the u_{nk} live in a common Hilbert space: that of periodic functions of period a. More about this, later on.

1.3. The adiabatic state: a glimpse at the adiabatic theorem

The problem we would like to study is the *time-dependent* Schrödinger equation

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = \widehat{H}(t)|\Psi(t)\rangle \ , \tag{1.8}$$

where $\widehat{H}(0) = \widehat{H}(T)$ and the period T is very long, i.e., the Hamiltonian changes slowly in time. In these circumstances, the adiabatic theorem helps us. To be general, let us assume that $\widehat{H}(t)$ depends on some n-dimensional set of parameters which we denote by $\mathbf{R}$, which are changed in time slowly and in a periodic fashion, $\widehat{H}(\mathbf{R}(t))$. Let us assume that the trajectory $\mathbf{R}(t)$ follows some curve $\mathbf{R}_s : s \in [0,1] \to \mathbf{R}_s \in \mathbb{R}^n$, with $\mathbf{R}(t) = \mathbf{R}_{s=t/T}$, i.e., we are rescaling the time t by the total time T, in such a way as to be able to control the overall "slowness" of the motion.

For every instantaneous value of $\mathbf{R}$, let us assume that we can find all eigenstates and eigenvalues of $\widehat{H}(\mathbf{R})$:

$$\widehat{H}(\mathbf{R})|\Phi_m(\mathbf{R})\rangle = E_m(\mathbf{R})|\Phi_m(\mathbf{R})\rangle \ . \tag{1.9}$$

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]

If you want to have a simple explicit example in mind, which will turn out to be crucially important in the following (incidentally, also the example that Berry addressed in his original paper [**?**]), you could think of $\widehat{H}(t)$ to represent a single spin-1/2 in a slowly varying magnetic field:

$$\widehat{H}(\mathbf{R}(t)) = g\mu_B \widehat{\mathbf{S}} \cdot \mathbf{B}(t) = \mathbf{R}(t) \cdot \hat{\boldsymbol{\sigma}} \ , \tag{1.10}$$

where we have reabsorbed a $g\mu_B/2 \approx \mu_B$ inside a general vectorial parameter $\mathbf{R}(t) = (g\mu_B/2)\mathbf{B}(t)$. $\mathbf{R}$ can 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:

$$|\Phi_{+\frac{1}{2}}(\mathbf{R})\rangle_N = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix} \qquad |\Phi_{-\frac{1}{2}}(\mathbf{R})\rangle_N = \begin{pmatrix} e^{-i\phi}\sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix} \ , \tag{1.11}$$

with corresponding energy $E_{\pm\frac{1}{2}} = \pm R$. Notice that $\mathbf{R}^* = \mathbf{0}$ is a degeneracy point in parameter space, where the gap between the two eigenstates closes. Notice also 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 $e^{\pm i\phi}$ is totally undetermined. We will see later on how this singularity reflects itself in the form of the Berry connection.

Assume that at the initial time the system is in some eigenstates, say $|\Phi_0(\mathbf{R}_0)\rangle$, and that the spectrum of eigenvalues is *non degenerate* and with a *gap*, i.e, every eigenvalue is separated

[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*.

from the other ones by a non vanishing quantity $E_n(\mathbf{R}) - E_m(\mathbf{R}) = \hbar\omega_{nm}$ with $|\omega_{nm}| > 0$. [4] The adiabatic theorem states that, if T is long enough, then the time dependent state $|\Psi(t)\rangle$ is close to the instantaneous state $|\Phi_0(\mathbf{R}(t))\rangle$. [5]

We will see a glimpse of the crucial ingredient in the proof below. A full proof, quite heavy to digest, is given in the book by Messiah [5, p. 747]. One of the non-trivial aspects of the story is that the *phase* accumulated by the state must have an extra piece, on top of the dynamical phase that you expect:

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

where the geometric phase $\gamma_0(t)$ — known as Berry phase — is necessary in order to have that

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

As you can verify with a simple calculation, this extra phase is given by

$$\gamma_0(t) \stackrel{def}{=} i\int_0^t dt' \ \dot{\mathbf{R}}(t')\cdot\langle\Phi_0(\mathbf{R}(t'))|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R}(t'))\rangle \ . \tag{1.12}$$

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 $\dot{\mathbf{R}}(t) = \frac{1}{T}\dot{\mathbf{R}}_s$. [6] Physically, you see that $\gamma_0(T)$ has a strict mechanical analogy in the *total work* done by the force field

$$\boldsymbol{\mathcal{A}}(\mathbf{R}) = i\langle\Phi_0(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R})\rangle = -\mathrm{Im}\langle\Phi_0(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R})\rangle \ , \tag{1.13}$$

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. More about it later on: here, it will play a rather minor role.

[4] In a condensed matter system all eigenvalues are extensive, i.e., they tend to infinity with the size of the system. Nevertheless, in an insulator, excitations cost a finite amount of energy, and this provides the necessary gap we are postulating.

[5] 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:

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

[6] 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 $g(1) = T$.

Unfortunately, the lowest order adiabatic result will not be sufficient for our purposes: we will have to derive the first-order correction into an adiabatic perturbation theory scheme. Let us see how it works. Assuming a completely general expansion of the form:

$$|\Psi(t)\rangle = \sum_m c_m(t)\, \mathrm{e}^{i\gamma_m(t)}\, \mathrm{e}^{-\frac{i}{\hbar}\int_0^t dt' E_m(\mathbf{R}(t'))}\, |\Phi_m(\mathbf{R}(t))\rangle\ , \tag{1.14}$$

it is rather simple to derive an exact differential equation that the unknown coefficients $c_m(t)$ have to satisfy:

$$\dot{c}_n(t) = \sum_{m\neq n} \mathrm{e}^{\frac{i}{\hbar}\int_0^t dt'(E_n - E_m)}\, F_{nm}(t)\, c_m(t)\ , \tag{1.15}$$

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

$$F_{nm}(t) = -\mathrm{e}^{i[\gamma_m(t)-\gamma_n(t)]}\, \langle \Phi_n(\mathbf{R}(t))|\partial_t \Phi_m(\mathbf{R}(t))\rangle\ . \tag{1.16}$$

The initial condition for this system of differential equations is $c_n(0) = \delta_{n,0}$. Hence, it is rather simple to understand that the most important term in the right-hand side is precisely the term with $n = 0$ (which starts from 1), while the other terms start having $c_m(t) \approx 0$ for small t. Hence, we can write the equation for $c_n(t)$, when $n \neq 0$, as follows:

$$\dot{c}_n(t) = (1-\delta_{n,0})\, \mathrm{e}^{\frac{i}{\hbar}\int_0^t dt'(E_n - E_0)}\, F_{n0}(t)\, c_0(t) + \sum_{m\neq(0,n)} (\cdots)$$

where the $(1-\delta_{n,0})$ term reminds us that $n \neq 0$ in that expression. Now, let us take one moment to comment on the effect of going slow, making $T \to \infty$. By implementing the change of variables to the rescaled time, $t \to s = t/T$, you immediately realize that the Schrödinger equation can be rewritten as:

$$i\hbar \frac{d}{ds}|\widetilde{\Psi}(s)\rangle = T\widehat{H}(\mathbf{R}_s)|\widetilde{\Psi}(s)\rangle\ , \tag{1.17}$$

where $|\widetilde{\Psi}(s)\rangle = |\Psi(t = sT)\rangle$. So, the whole role of T is to multiply the Hamiltonian, hence the instantaneous eigenvalues $E_n(\mathbf{R}_s)$. Formally, in the rescaled time s you might rewrite the previous equation for the coefficient c_n as follows:

$$\dot{c}_n(s) = (1-\delta_{n,0})\, \mathrm{e}^{\frac{iT}{\hbar}\int_0^s ds'(E_n - E_0)}\, F_{n0}(s)\, c_0(s) + \sum_{m\neq(0,n)} (\cdots)\ .$$

And now you realize that a large factor T in the exponential makes the phase factor wildly oscillatory, provided $|E_n - E_0| > 0$. If you want to see that this wild oscillation makes the contribution small, simply integrate by parts the exponential. [7] You will write something like:

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

showing that the coefficients $c_{n\neq 0}$ have an overall factor $1/T$ in front. And this is not all. The gap ω_{n0} appears in the denominator. But if you examin more closely the F_{n0}, you discover an extra factor of ω_{n0} coming out of it. Let us examine in detail $F_{n0}(s)$:

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

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

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. (1.9), and taking the scalar product with $\langle\Phi_n|$, it is immediate to prove that:

$$\langle\Phi_n(\mathbf{R}_s)|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R}_s)\rangle = -\frac{\langle\Phi_n(\mathbf{R}_s)|\boldsymbol{\nabla}_{\mathbf{R}}\widehat{H}|\Phi_0(\mathbf{R}_s)\rangle}{E_n(\mathbf{R}_s) - E_0(\mathbf{R}_s)} \,, \tag{1.18}$$

which, upon substitution in F_{n0} gives:

$$F_{n0}(s) = \mathrm{e}^{i[\gamma_0(s)-\gamma_n(s)]}\, \frac{\dot{\mathbf{R}}_s \cdot \langle\Phi_n(\mathbf{R}_s)|\boldsymbol{\nabla}_{\mathbf{R}}\widehat{H}|\Phi_0(\mathbf{R}_s)\rangle}{E_n(\mathbf{R}_s) - E_0(\mathbf{R}_s)} \,. \tag{1.19}$$

So, the larger (in modulus) is the gap $\hbar\omega_{n0} = E_n - E_0$, the smaller is F_{n0}. One might be tempted to even put down a *condition for adiabaticity* by requiring the smallness of the first term, i.e., for all $s \in [0,1]$:

$$\left|\frac{F_{n0}(s)}{T\omega_{n0}(s)}\right| = \left|\frac{\hbar}{T}\,\frac{\dot{\mathbf{R}}_s \cdot \langle\Phi_n(\mathbf{R}_s)|\boldsymbol{\nabla}_{\mathbf{R}}\widehat{H}|\Phi_0(\mathbf{R}_s)\rangle}{[E_n(\mathbf{R}_s) - E_0(\mathbf{R}_s)]^2}\right| \ll 1 \,. \tag{1.20}$$

Let us now return to our usual time t, and make a perturbation theory expansion up to first order. Hence, to zeroth order we take $c_n^{(0)}(t) = \delta_{n,0}$, and plug this into the right-hand side of 1.15, obtaining the solution up to first-order in the form:

$$\dot{c}_n^{(1)}(t) = (1-\delta_{n0})\, \mathrm{e}^{i\int_0^t dt'\omega_{n0}}\, F_{n0}(t) \,. \tag{1.21}$$

Notice that there are no corrections to c_0 at first order. Now, as previously done to show the crucial ingredient behind the adiabatic theorem, integrate this equation by parts and neglect all terms which contain derivatives (because they come with an extra factor $1/T$):

$$c_n^{(1)}(t) = (1-\delta_{n0})\, \frac{\mathrm{e}^{i\int_0^t dt'\omega_{n0}}}{i\omega_{n0}}\, F_{n0}(t) \;+\; \text{derivative terms} \,. \tag{1.22}$$

Inserting this expression in the expansion of the state, we can finally write an approximate expression for $|\Psi(t)\rangle$, to first-order in the time-derivatives, as follows:

$$|\Psi(t)\rangle = \mathrm{e}^{i\gamma_0(t)}\, \mathrm{e}^{-\frac{i}{\hbar}\int_0^t dt' E_0(t')} \left[|\Phi_0(t)\rangle + i\hbar \sum_{n\neq 0} \frac{|\Phi_n(t)\rangle\langle\Phi_n(t)|\partial_t\Phi_0(t)\rangle}{E_n(t) - E_0(t)}\right] , \tag{1.23}$$

which coincides with Eq. (2.3) of Ref. [1]. The second term contains an important correction to the adiabatic state which will play a crucial role in transport, as we shall presently see.

1.4. The pumped charge and its topological features

Now we have all the ingredients to calculate the pumped charge Q. Let us start from the average current $\langle\Psi(t)|\widehat{J}|\Psi(t)\rangle$. With the results derived so far we can write:

$$\langle\Psi(t)|\widehat{J}|\Psi(t)\rangle = \langle\Phi_0(t)|\frac{1}{\hbar}\partial_\kappa\hat{H}(t)|\Phi_0(t)\rangle + i\sum_{n\neq 0}\left[\frac{\langle\Phi_0(t)|\partial_\kappa\hat{H}(t)|\Phi_n(t)\rangle\langle\Phi_n(t)|\partial_t\Phi_0(t)\rangle}{E_n(t) - E_0(t)} - \text{c.c.}\right] ,$$

where "c.c." is an abbreviation for the complex conjugate. In the second term we have kept the correction to the adiabatic state only once. Notice that the correction is "small" in the adiabatic limit: of order $1/T$. However, this correction will make up for the whole interesting part of the story, since when integrated over time in $[0, T]$ it will indeed give a non-vanishing (topological) contribution. Recall that we will have to set $\kappa = 0$ at the end, and that all eigenstates are calculated for given κ (although not explicitly indicated). The first term can be calculated through the Hellmann-Feynman theorem, which guarantees that

$$\langle \Phi_0(t)|\partial_\kappa \hat{H}(t)|\Phi_0(t)\rangle = \partial_\kappa \langle \Phi_0(t)|\hat{H}(t)|\Phi_0(t)\rangle = \partial_\kappa E_0(t) \ .$$

In the second term we can substitute [8]

$$\frac{\langle \Phi_0(t)|\partial_\kappa \hat{H}(t)|\Phi_n(t)\rangle}{E_n(t) - E_0(t)} = -\langle \partial_\kappa \Phi_0(t)|\Phi_n(t)\rangle \ ,$$

valid for all $n \neq 0$. Whence we get:

$$\begin{aligned} \langle \Psi(t)|\widehat{J}|\Psi(t)\rangle &= \frac{1}{\hbar}\partial_\kappa E_0(\kappa,t) - i\sum_{n\neq 0}\Big[\langle \partial_\kappa \Phi_0(t)|\Phi_n(t)\rangle\langle \Phi_n(t)|\partial_t \Phi_0(t)\rangle - \text{c.c.}\Big] \\ &= \frac{1}{\hbar}\partial_\kappa E_0(\kappa,t) - i\Big[\langle \partial_\kappa \Phi_0(t)|\partial_t \Phi_0(t)\rangle - \text{c.c.}\Big] \ , \end{aligned} \tag{1.24}$$

where in the final step we have used the fact that a term with $n = 0$ can be freely added because it is *real*,[9] hence it cancels when you subtract the complex conjugate; hence the whole unrestricted sum over n can be eliminated, since it gives the identity.

So far, we did not assume that the system was a band insulator. Suppose now that we can treat the interaction in some mean-field way, within the usual approach of the band-theory of crystals. Then the ground state $|\Phi_0\rangle$ would be (for fermionic systems) a *Slater determinant* of Bloch waves. If we work with the periodic functions $u_{n,k}(x,t)$, you might write it (in a second-quantization form) as

$$|\Phi_0(t)\rangle = \prod_{\nu}^{\text{occ}}\prod_{k_n}^{\text{BZ}} \hat{c}^\dagger_{\nu,k_n}(t)\ |0\rangle \ ,$$

where $\hat{c}^\dagger_{\nu,k}(t)$ creates a particle in the instantaneous (i.e., at fixed value of t) state $u_{\nu,k}(x,t) = \langle x|\hat{c}^\dagger_{\nu,k}(t)|0\rangle$. Here k_n indicate all the wave-vector of a discretization of the BZ (assuming we have a very large system of size $L = Na$ with PBC applied, $k_n = 2\pi n/L$ with $n = -N/2+1, \cdots, N/2$). While we might sometimes omit the dependence on t, we should always remember that we are assuming a *fixed* value of t. Recall that the (single-particle) Hamiltonian which governs the $u_{\nu,k}$ have an explicit momentum dependence in the kinetic

[8] It is simple to derive this relationship. Start from $\hat{H}(t)|\Phi_n(t)\rangle = E_n(t)|\Phi_n(t)\rangle$, apply a derivative with respect to κ and take the scalar product with $\langle \Phi_0|$ (assuming $n \neq 0$).

[9] Notice that $\langle \partial_\kappa \Phi_0|\Phi_0\rangle$ is purely imaginary, since:

$$\langle \partial_\kappa \Phi_0|\Phi_0\rangle + \langle \Phi_0|\partial_\kappa \Phi_0\rangle = \partial_\kappa \langle \Phi_0|\Phi_0\rangle = 0 \ .$$

energy $\widehat{H}(k,t) = (\hat{p}+\hbar k)^2/(2m) + v(x,t)$. In the presence of the extra flux, it would also acquire an extra piece $\hbar\kappa$:

$$\widehat{H}(k,\kappa,t) = \frac{(\hat{p}+\hbar k+\hbar\kappa)^2}{2m} + v(x,t) \; .$$

From there you see that everything depends only on $k+\kappa$, so that the total energy of the Slater determinant in the presence of κ would be:

$$E_0(\kappa,t) = \sum_{\nu}^{\rm occ}\sum_{k_n}^{\rm BZ} \epsilon_{\nu,k_n+\kappa}(t) \; .$$

From there you see that the total current associated to $|\Phi_0\rangle$, taking a derivative and setting $\kappa = 0$, would be:

$$\langle\Phi_0|\widehat{J}|\Phi_0\rangle = \sum_{\nu}^{\rm occ}\sum_{k_n}^{\rm BZ} \frac{1}{\hbar}\frac{\partial\epsilon_{\nu,k}}{\partial k}\Big|_{k=k_n} = 0 \; .$$

The reason is simple: the contribution to the current from each wave of momentum k is given by the group velocity $\partial_k\epsilon_{\nu,k}$ but there are cancellations between positive and negative momenta: in particular, this is rather obvious in an insulator, where all k's in the BZ are occupied, and there are no partially filled bands. Notice that this would be true for any given fixed time t.

Let us now see how the second term in Eq. 1.24 looks like for a band insulator. If you have a *single* particle in some band state $u_{\nu,k}(x,t)$, then

$$\langle\partial_\kappa\Phi_0(t)|\partial_t\Phi_0(t)\rangle\Big|_{\kappa=0} = \langle\partial_k u_{\nu,k}|\partial_t u_{\nu,k}\rangle \; .$$

More generally, if you have a certain number of bands fully occupied for all the momenta k in the BZ, a simple application of second quantization (or directly with Slater determinants) shows that you will get:

$$\langle\partial_\kappa\Phi_0(t)|\partial_t\Phi_0(t)\rangle\Big|_{\kappa=0} = \sum_{\nu}^{\rm occ}\sum_{k}^{\rm BZ}\langle\partial_k u_{\nu,k}|\partial_t u_{\nu,k}\rangle \; .$$

Putting all the ingredients together, we finally arrived at the following expression for the average current:

$$\langle\Psi(t)|\widehat{J}|\Psi(t)\rangle = -i\sum_{\nu}^{\rm occ}\sum_{k}^{\rm BZ}\Big[\langle\partial_k u_{\nu,k}|\partial_t u_{\nu,k}\rangle - \text{c.c.}\Big] \; . \tag{1.25}$$

Notice that the sum over the (discretized) wave-vectors k runs over the $N = L/a$ points in the BZ: this clearly shows that the total current is *extensive*, i.e., proportional to L. To get the "charge" that passes, during a period $[0,T]$, from one side of the sample to the other, you have to divide the current by L (taking the limit $L\to\infty$), and integrate it over time:

$$\begin{aligned} Q &= \lim_{L\to\infty}\frac{1}{L}\int_0^T dt\,\langle\Psi(t)|\widehat{J}|\Psi(t)\rangle = \\ &= -\sum_{\nu}^{\rm occ}\int_{-\frac{\pi}{a}}^{+\frac{\pi}{a}}\frac{\mathrm{d}k}{2\pi}\int_0^T dt\,\underbrace{i\Big[\langle\partial_k u_{\nu,k}|\partial_t u_{\nu,k}\rangle - \text{c.c.}\Big]}_{\mathcal{B}^{\nu}_{k,t}} \; , \end{aligned} \tag{1.26}$$

where the sum over the k's has been transformed into an integral [10] in the limit $L \to \infty$. The final expression for Q we got is the crucial goal of our long journey. It involves a double integral, over k and t, of an object that will be the main actor in the discussion of the Berry phase, the Berry curvature of the ν-th band:

$$\mathcal{B}^{\nu}_{k,t}(k,t) = i\Big[\langle \partial_k u_{\nu,k} | \partial_t u_{\nu,k}\rangle - \text{c.c.}\Big] \,. \tag{1.27}$$

The notation is here a bit reduntant, as k, t appear both as pedices of $\mathcal{B}$ (to recall the order in which you take the derivatives of $u_{\nu,k}$ in the anti-symmetric combination shown above), and as variables, because $\mathcal{B}$ depends on the point k, t on which you calculate it. But the crucial aspect of the story is that the integration you should perform is on the two-dimensional torus in (k, t) space, as both the BZ and the time-integral involve a periodic identification of their end-points. A proof that the integral of $\mathcal{B}^{\nu}_{k,t}$ over the torus in (k, t) space gives necessarily an *integer*, is one of the key-points in Ref. [1]. An explicit proof, making use of Stokes' theorem, is reported in Ref. [6][Sec. IIB]. We will not present it explicitly in class simply because the fact that Q is an integer, does not show that this integer is *different from* 0. In order to show that this integer can be non-trivial, i.e., $Q \neq 0$, we will resort to an explicit calculation within a tight-binding approximation, leading to the Rice-Mele model discussed later on.

[10] This follows from thinking the integral in terms of discrete Riemann sums, with the width of the rectangles which discretize the integral being all equal to $2\pi/L$. Hence:

$$\lim_{L\to\infty} \frac{1}{L} \sum_{k}^{\text{BZ}} f(k) = \int_{-\frac{\pi}{a}}^{+\frac{\pi}{a}} \frac{\mathrm{d}k}{2\pi}\, f(k) \,.$$

2. Berry phase

I present in this chapter the essential properties of the so-called Berry phase [7] 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. [8, Chap. 5].

The appearence of the geometric phase within a context of adiabatic dynamics and adiabatic theorem is briefly presented in Sec. 1.3.

2.1. Berry phase: generalities

Let us explore another route to get the geometrical phase we have found in discussing the adiabatic theorem. 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 space with $s_j \in [0,1]$, $j = 0, \ldots P$, 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:

$$\begin{aligned}\Delta\phi_{j,j+1} &= -\mathrm{Im}\log\langle\Phi_0(\mathbf{R}_{s_j})|\Phi_0(\mathbf{R}_{s_{j+1}})\rangle \\ &= -\mathrm{Im}\log\left(1+\langle\Phi_0(\mathbf{R}_{s_j})|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R}_{s_j})\rangle\cdot\Delta\mathbf{R}+\cdots\right) \\ &= i\langle\Phi_0(\mathbf{R}_{s_j})|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R}_{s_j})\rangle\cdot\Delta\mathbf{R}+\cdots\ , \end{aligned} \tag{2.1}$$

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:

$$\boldsymbol{\mathcal{A}}(\mathbf{R})=i\langle\Phi_0(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R})\rangle=-\mathrm{Im}\langle\Phi_0(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R})\rangle\ . \tag{2.2}$$

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

$$\boldsymbol{\mathcal{A}}'=\boldsymbol{\mathcal{A}}+\boldsymbol{\nabla}_{\mathbf{R}}\Lambda(\mathbf{R})\ , \tag{2.3}$$

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 [8, 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:

$$\boldsymbol{\mathcal{B}}(\mathbf{R})=\boldsymbol{\nabla}_{\mathbf{R}}\times\boldsymbol{\mathcal{A}}(\mathbf{R})=-\mathrm{Im}\langle\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R})|\times|\boldsymbol{\nabla}_{\mathbf{R}}\Phi_0(\mathbf{R})\rangle\ , \tag{2.4}$$

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:

$$\gamma=\oint_{\partial\Sigma}\boldsymbol{\mathcal{A}}(\mathbf{R})\cdot d\mathbf{R}=\int_\Sigma\boldsymbol{\mathcal{B}}(\mathbf{R})\cdot\mathbf{n}\ d\sigma\ . \tag{2.5}$$

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 $\boldsymbol{\mathcal{B}}(\mathbf{R})$ read:

$$\mathcal{B}_1(\mathbf{R})=-\mathrm{Im}\Big[\langle\partial_2\Phi_0(\mathbf{R})|\partial_3\Phi_0(\mathbf{R})\rangle-\langle\partial_3\Phi_0(\mathbf{R})|\partial_2\Phi_0(\mathbf{R})\rangle\Big]\ , \tag{2.6}$$

and similar equations for $\mathcal{B}_2$ and $\mathcal{B}_3$ 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:

$$\mathcal{B}_1(\mathbf{R}) = i\Big[\langle\partial_2\Phi_0(\mathbf{R})|\partial_3\Phi_0(\mathbf{R})\rangle - \langle\partial_3\Phi_0(\mathbf{R})|\partial_2\Phi_0(\mathbf{R})\rangle\Big] = -2\mathrm{Im}\langle\partial_2\Phi_0(\mathbf{R})|\partial_3\Phi_0(\mathbf{R})\rangle \ . \quad (2.7)$$

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:

$$\mathcal{B}_{\alpha\beta}(\mathbf{R}) = -2\mathrm{Im}\langle\partial_\alpha\Phi_0(\mathbf{R})|\partial_\beta\Phi_0(\mathbf{R})\rangle = i\Big[\langle\partial_\alpha\Phi_0(\mathbf{R})|\partial_\beta\Phi_0(\mathbf{R})\rangle - \langle\partial_\beta\Phi_0(\mathbf{R})|\partial_\alpha\Phi_0(\mathbf{R})\rangle\Big] \ , \quad (2.8)$$

the only difference being that in general this object has more components, $n(n-1)/2$ for general $n > 1$. By construction $\mathcal{B}_{\alpha\beta} = -\mathcal{B}_{\beta\alpha}$, hence $\mathcal{B}_{\alpha\alpha} = 0$. [1] 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 $\mathcal{B}_{\alpha\beta}(\mathbf{R})$ as follows:

$$\mathcal{B}_{\alpha\beta}(\mathbf{R}) = -2\mathrm{Im}\langle\partial_\alpha\Phi_0(\mathbf{R})|\mathbb{Q}(\mathbf{R})|\partial_\beta\Phi_0(\mathbf{R})\rangle \ . \quad (2.9)$$

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:

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

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 $\boldsymbol{\mathcal{B}}$ plays the role of a magnetic field. [2]

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

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

$$\mathcal{G}_{\alpha\beta}(\mathbf{R}) = \langle\partial_\alpha\Phi_0(\mathbf{R})|\mathbb{Q}(\mathbf{R})|\partial_\beta\Phi_0(\mathbf{R})\rangle \ , \quad (2.10)$$

of which $\mathcal{B}_{\alpha\beta}$ 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].

We are now in the position to write a further expression for $\mathcal{B}_{\alpha\beta}(\mathbf{R})$, perhaps mathematically less elegant, but still physically very useful. If you recall that discussion on the adiabatic theorem, see Eq. (1.18), you will remember that for all states with $E_n \neq E_0$ we have (in the new notation): [3]

$$\langle \Phi_n(\mathbf{R}) | \partial_\beta \Phi_0(\mathbf{R}) \rangle = \frac{\langle \Phi_n(\mathbf{R}) | \partial_\beta \widehat{H} | \Phi_0(\mathbf{R}) \rangle}{E_0(\mathbf{R}) - E_n(\mathbf{R})} \ . \tag{2.13}$$

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

$$\begin{aligned} \mathcal{B}_{\alpha\beta}(\mathbf{R}) &= -2\mathrm{Im} \sum_{n\neq 0} \langle \partial_\alpha \Phi_0(\mathbf{R}) | \Phi_n(\mathbf{R}) \rangle \langle \Phi_n(\mathbf{R}) | \partial_\beta \Phi_0(\mathbf{R}) \rangle \\ &= -2\mathrm{Im} \sum_{n\neq 0} \frac{\langle \Phi_0(\mathbf{R}) | \partial_\alpha \widehat{H} | \Phi_n(\mathbf{R}) \rangle \langle \Phi_n(\mathbf{R}) | \partial_\beta \widehat{H} | \Phi_0(\mathbf{R}) \rangle}{[E_0(\mathbf{R}) - E_n(\mathbf{R})]^2} \ . \end{aligned} \tag{2.14}$$

This expression for $\mathcal{B}_{\alpha\beta}$, involving standard energy denominators, often appears in physical calculations and also reveals some interesting aspects related to singularities of $\mathcal{B}_{\alpha\beta}(\mathbf{R})$. In particular, on notices that $\mathcal{B}_{\alpha\beta}(\mathbf{R})$ is singular whenever the gap between E_n and E_0 closes at some point $\mathbf{R}^*$, which might be away from your physical trajectory $\mathbf{R}(t)$, but will nevertheless have important physical implications. One of the important advantages of it is the fact that it does not involve any derivative of the *states*, hence it can be calculated with any phase choice for the states, including choices that are not smooth (as, for instance, when the eigenstates are obtained numerically).

2.2. 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:

$$\widehat{H}(\mathbf{B}(t)) = -g\mu \widehat{\mathbf{S}} \cdot \mathbf{B}(t) \ , \tag{2.15}$$

[3] 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:

$$|\Phi_n(\lambda)\rangle = |\Phi_n(0)\rangle + \lambda \sum_{m\neq n} |\Phi_m(0)\rangle \frac{\langle \Phi_m(0) | \hat{V} | \Phi_n(0) \rangle}{E_n(0) - E_m(0)} + O(\lambda^2) \ . \tag{2.11}$$

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

$$\langle \Phi_m(0) | \partial_\lambda \Phi_n(\lambda) \rangle \Big|_{\lambda=0} = \frac{\langle \Phi_m(0) | \partial_\lambda \hat{H}(\lambda) | \Phi_n(0) \rangle}{E_n(0) - E_m(0)} \Big|_{\lambda=0} \ , \tag{2.12}$$

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.

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:

$$\mathcal{B}^{(m)}_{\alpha\beta}(\mathbf{B}) = -2\mathrm{Im}\sum_{m'\neq m}\frac{\langle\Phi_m(\mathbf{B})|\widehat{S}_\alpha|\Phi_{m'}(\mathbf{B})\rangle\langle\Phi_{m'}(\mathbf{B})|\widehat{S}_\beta|\Phi_m(\mathbf{B})\rangle}{B^2[m-m']^2}\,, \tag{2.16}$$

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:

$$\mathcal{B}^{(m)}_{x'y'}(\mathbf{B}) = -2\mathrm{Im}\sum_{m'\neq m}\frac{\langle\Phi_m(\mathbf{B})|\widehat{S}_{x'}|\Phi_{m'}(\mathbf{B})\rangle\langle\Phi_{m'}(\mathbf{B})|\widehat{S}_{y'}|\Phi_m(\mathbf{B})\rangle}{B^2[m-m']^2}\,. \tag{2.17}$$

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:

$$\mathcal{B}^{(m)}_{x'y'}(\mathbf{B}) = -\frac{m}{B^2}\,, \tag{2.18}$$

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 $\boldsymbol{\mathcal{B}}$ which is in the radial direction $\mathbf{B}$ and proportional to $-m/B^2$:

$$\boldsymbol{\mathcal{B}}^{(m)}(\mathbf{B}) = -m\frac{\hat{\mathbf{B}}}{B^2}\,. \tag{2.19}$$

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:

$$\gamma_m(C) = \int_{\Sigma_C}\boldsymbol{\mathcal{B}}^{(m)}(\mathbf{B})\cdot\mathbf{n}\,d\sigma = -m\int_{\Sigma_C}\frac{\hat{\mathbf{B}}}{B^2}\cdot\hat{\mathbf{B}}\;B^2\,d\Omega = -m\Omega(C)\,, \tag{2.20}$$

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

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

Let us consider in more detail the case $S = 1/2$ which will occur very often in the discussion of the different models we will tackle. 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 that of a spin-1/2 electron in a magnetic field

$$\widehat{H}(\mathbf{R}(t)) = g\mu_B \widehat{\mathbf{S}}\cdot\mathbf{B}(t) = \mathbf{R}(t)\cdot\hat{\boldsymbol{\sigma}}\ , \tag{2.21}$$

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:

$$|\Phi_{+\frac{1}{2}}(\mathbf{R})\rangle_N = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix} \qquad |\Phi_{-\frac{1}{2}}(\mathbf{R})\rangle_N = \begin{pmatrix} e^{-i\phi}\sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix}\ , \tag{2.22}$$

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 $e^{\pm i\phi}$ 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 $e^{\mp i\phi}$, giving:

$$|\Phi_{+\frac{1}{2}}(\mathbf{R})\rangle_S = \begin{pmatrix} e^{-i\phi}\cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix} \qquad |\Phi_{-\frac{1}{2}}(\mathbf{R})\rangle_S = \begin{pmatrix} \sin\frac{\theta}{2} \\ -e^{i\phi}\cos\frac{\theta}{2} \end{pmatrix}\ , \tag{2.23}$$

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:

$$\boldsymbol{\mathcal{A}} = \mathcal{A}_R\widehat{\mathbf{R}} + \mathcal{A}_\theta\widehat{\boldsymbol{\theta}} + \mathcal{A}_\phi\widehat{\boldsymbol{\phi}}\ , \tag{2.24}$$

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

$$\begin{aligned}
\mathcal{A}^{(N)}_{R,\pm} &= i\langle\Phi_{\pm\frac{1}{2}}|\partial_R\Phi_{\pm\frac{1}{2}}\rangle_N = 0 \\
\mathcal{A}^{(N)}_{\theta,\pm} &= \frac{1}{R}i\langle\Phi_{\pm\frac{1}{2}}|\partial_\theta\Phi_{\pm\frac{1}{2}}\rangle_N = 0 \\
\mathcal{A}^{(N)}_{\phi,\pm} &= \frac{1}{R\sin\theta}i\langle\Phi_{\pm\frac{1}{2}}|\partial_\phi\Phi_{\pm\frac{1}{2}}\rangle_N = \mp\frac{\sin^2\frac{\theta}{2}}{R\sin\theta} = \mp\frac{1-\cos\theta}{2R\sin\theta}\ ,
\end{aligned} \tag{2.25}$$

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

$$\begin{aligned}
\mathcal{A}^{(S)}_{R,\pm} &= i\langle\Phi_{\pm\frac{1}{2}}|\partial_R\Phi_{\pm\frac{1}{2}}\rangle_S = 0 \\
\mathcal{A}^{(S)}_{\theta,\pm} &= \frac{1}{R}i\langle\Phi_{\pm\frac{1}{2}}|\partial_\theta\Phi_{\pm\frac{1}{2}}\rangle_S = 0 \\
\mathcal{A}^{(S)}_{\phi,\pm} &= \frac{1}{R\sin\theta}i\langle\Phi_{\pm\frac{1}{2}}|\partial_\phi\Phi_{\pm\frac{1}{2}}\rangle_S = \pm\frac{\cos^2\frac{\theta}{2}}{R\sin\theta} = \pm\frac{1+\cos\theta}{2R\sin\theta}\ ,
\end{aligned} \tag{2.26}$$

with a vortex singularity at the North pole.

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

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

This immediately gives:

$$\mathcal{B}_\pm = \frac{\widehat{\mathbf{R}}}{R\sin\theta}\left[\partial_\theta\left(\mp\frac{1-\cos\theta}{2R}\right)\right] = \mp\frac{1}{2}\frac{\widehat{\mathbf{R}}}{R^2} , \tag{2.27}$$

which coincides with Eq. (2.19) for $m = \pm\frac{1}{2}$. This $\mathcal{B}$ 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 $\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}$. [4] To be more precise, one cannot find a single $\mathbf{A}$ 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:

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

[4] 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 $\boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} \times \mathbf{A}) = 0$.

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:

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

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:

$$\begin{aligned} \mathbf{A}^{(N)} &= \frac{e_M}{R}\frac{1-\cos\theta}{\sin\theta}\,\widehat{\boldsymbol{\phi}} \\ \mathbf{A}^{(S)} &= -\frac{e_M}{R}\frac{1+\cos\theta}{R\sin\theta}\,\widehat{\boldsymbol{\phi}}\,. \end{aligned} \tag{2.28}$$

I plot them in Fig. 2.1. Observe that the two choices are related by a gauge transformation $\Lambda = 2e_M\phi$:

$$\mathbf{A}^{(N)} - \mathbf{A}^{(S)} = 2e_M\frac{1}{R\sin\theta}\,\widehat{\boldsymbol{\phi}} = \boldsymbol{\nabla}\Lambda = \boldsymbol{\nabla}(2e_M\phi)\,. \tag{2.29}$$

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, [5] 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:

$$\psi^{(S)}(\mathbf{R}) = \exp\left(-i\frac{2ee_M}{\hbar c}\phi\right)\psi^{(N)}(\mathbf{R})\,. \tag{2.30}$$

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:

$$\frac{2ee_M}{\hbar c} = n \qquad \text{with } n = 0, \pm1, \pm2, \cdots \tag{2.31}$$

[5] 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.

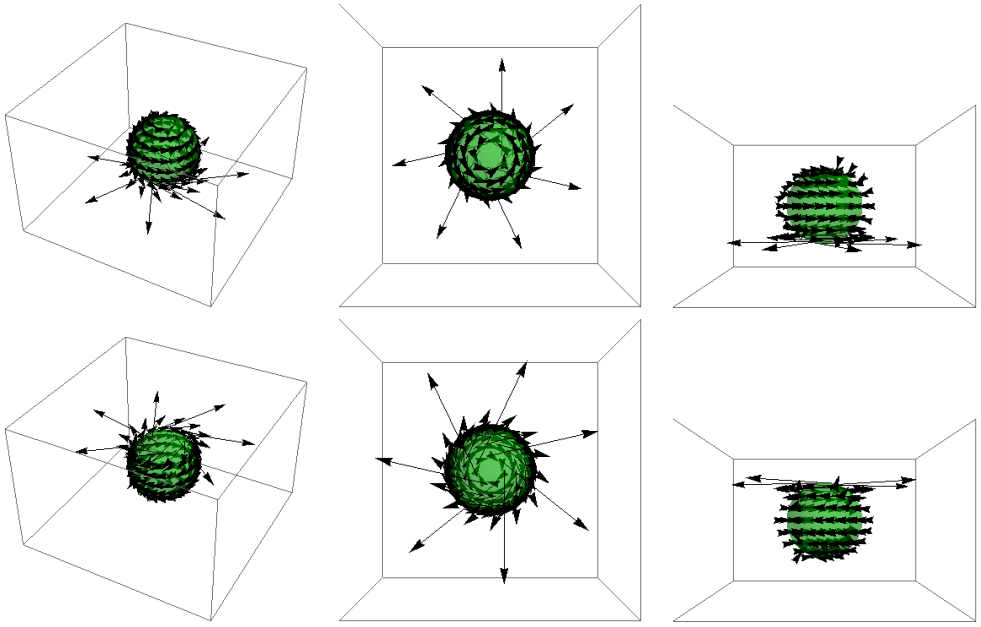

Figure 2.1.: Two of the possible choices of monopole vector potentials: $A^{(N)}$ (top, including a view from above and a front view) which is regular at the North pole and with a vortex at the south pole, and $A^{(S)}$ (bottom), vice-versa. Notice the opposite direction of rotation of the arrows in the two cases.

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 calculation by saying that:

$$\begin{aligned}
\int_{\Sigma_N} \mathbf{B}\cdot\mathbf{n}\, d\sigma &= \int_C \mathbf{A}^{(N)}\cdot d\mathbf{R} \\
\int_{\Sigma_S} \mathbf{B}\cdot\mathbf{n}\, d\sigma &= -\int_C \mathbf{A}^{(S)}\cdot d\mathbf{R} \\
\int_{S^2} \mathbf{B}\cdot\mathbf{n}\, d\sigma &= \int_C [\mathbf{A}^{(N)}-\mathbf{A}^{(S)}]\cdot d\mathbf{R} = \int_C 2e_M \boldsymbol{\nabla}\phi\cdot d\mathbf{R} = 4\pi e_M\ .
\end{aligned} \tag{2.32}$$

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 $\Lambda = 2e_M\phi$.

3. Thouless adiabatic pump: tight-binding approaches

Until now, we have set up the problem of Thouless pumping on the continuum. But the fact that any charge is transported is still not clear: after all, 0 is an integer, and the interesting things would be to have a *non trivial* integer with $Q \neq 0$. In order to see that such non-trivial cases are possible, let us do an explicit realization where the calculations can be easily performed, but within a tight-binding approximation. The tight-binding approximation relies on switching from the basis of Bloch states, to a basis of Wannier orbitals centered on the different sites of the potential $v(x,t)$. We will consider a situation in which the parameters (mass m of the atoms, wavelength λ of the laser, determining the period d_s of the standing wave $V_s(x)$ and the confining kinetic energy $\hbar^2/(2md_s^2)$ and the height of the barriers) are such that you expect that a single wannier orbital is important and relevant in each valley of the potential. Let us denote this Wannier orbital by $w_{jA}(x)$ and $w_{jB}(x)$, where the notation is such that each valley is labelled as $j, A/B$ where $j = 1 \cdots N$ denotes the periodicity unit cell, and A/B the sublattice index referring to which of the two valleys in the unit cell we consider. Let us write down, right away, a tight-binding model which describes such physical situation: it is a model introduced long ago by Rice and Mele.

3.1. The Rice-Mele model

The Rice-Mele model can be written as follows:

$$\hat{H}_{\mathrm{RM}} = -J_1 \sum_{j=1}^{N} \left(\hat{c}^\dagger_{j,B} \hat{c}_{j,A} + \mathrm{H.c.} \right) - J_2 \sum_{j=1}^{N} \left(\hat{c}^\dagger_{j+1,A} \hat{c}_{j,B} + \mathrm{H.c.} \right) + \sum_{j=1}^{N} \left(\epsilon_A \hat{n}_{j,A} + \epsilon_B \hat{n}_{j,B} \right) \quad (3.1)$$

Let us start assuming that periodic boundary conditions (PBC) are used, in such a way that $\hat{c}^\dagger_{N+1,A/B} \equiv \hat{c}^\dagger_{1,A/B}$, i.e., the cell number $N+1$ coincides with cell number 1 (or equivalently, you can visualize your system as being on a ring). The parameters J_1 (intra-cell hopping), J_2 (inter-cell hopping) and $\epsilon_{A/B}$ (the on-site energy of the Wannier orbital $w_{j,A/B}$) clearly depend on the phase difference φ, which in turn depends on time as $\varphi(t) = 2\pi t/T$. Hence, in the end, what we have is a *time-dependent* non-interacting Hamiltonian $\hat{H}_{\mathrm{RM}}(t)$, where the dependence on t comes through the parameters $J_1(\varphi(t))$, $J_2(\varphi(t))$, $\epsilon_{A/B}(\varphi(t))$. To simplify

the problem a bit, let us assume that the parameters depend on time as follows:

$$\begin{aligned} J_1(t) &= J_0 + \delta_0 \cos\frac{2\pi t}{T} = J_0 + \delta(t) \\ J_2(t) &= J_0 - \delta_0 \cos\frac{2\pi t}{T} = J_0 - \delta(t) \\ \epsilon_A(t) &= \epsilon_0 + \Delta_0 \sin\frac{2\pi t}{T} = \epsilon_0 + \Delta(t) \\ \epsilon_B(t) &= \epsilon_0 - \Delta_0 \sin\frac{2\pi t}{T} = \epsilon_0 + \Delta(t)\ . \end{aligned} \tag{3.2}$$

Hence, setting the zero of energy in such a way that $\epsilon_0 = 0$ we can rewrite our model as:

$$\begin{aligned} \hat{H}_{\rm RM}(t) &= -(J_0+\delta(t))\sum_{j=1}^{N}\left(\hat{c}^\dagger_{j,B}\hat{c}_{j,A} + \text{H.c.}\right) - (J_0-\delta(t))\sum_{j=1}^{N}\left(\hat{c}^\dagger_{j+1,A}\hat{c}_{j,B} + \text{H.c.}\right) \\ &\quad +\Delta(t)\sum_{j=1}^{N}\left(\hat{n}_{j,A} - \hat{n}_{j,B}\right)\ . \end{aligned} \tag{3.3}$$

When periodic boundary conditions (PBC) are applied, one can exploit translational invariance, defining the Bloch-Wannier transformations:

$$\begin{cases} \hat{c}^\dagger_{k,A} = \dfrac{1}{\sqrt{N}}\displaystyle\sum_{j=1}^{N} \mathrm{e}^{ikaj}\hat{c}^\dagger_{j,A} \\ \hat{c}^\dagger_{k,B} = \dfrac{1}{\sqrt{N}}\displaystyle\sum_{j=1}^{N} \mathrm{e}^{ikaj}\hat{c}^\dagger_{j,B} \end{cases} \qquad \begin{cases} \hat{c}^\dagger_{j,A} = \dfrac{1}{\sqrt{N}}\displaystyle\sum_{k}^{\rm BZ} \mathrm{e}^{-ikaj}\hat{c}^\dagger_{k,A} \\ \hat{c}^\dagger_{j,B} = \dfrac{1}{\sqrt{N}}\displaystyle\sum_{k}^{\rm BZ} \mathrm{e}^{-ikaj}\hat{c}^\dagger_{k,B} \end{cases} . \tag{3.4}$$

Here N is the number of unit cells making-up a big periodically-repeated lattice of length $L = Na$ (i.e., wrapped-up on a circle): as a consequence, the *discrete* wave-vectors allowed are

$$k = \frac{2\pi n}{Na} = \frac{2\pi n}{L} \qquad \text{with} \quad n \in \mathbb{Z}\ , \tag{3.5}$$

with the understanding that only N of them are independent; for instance $n = 0 \cdots N-1$, or $n = -N/2+1, \cdots N/2$, making up the first Brillouin Zone (BZ) of the reciprocal lattice. Inserting these expressions into the Rice-Mele model, we can transform it in the form:

$$\hat{H}_{\rm RM}(t) = \sum_{k}^{\rm BZ}\left[\hat{c}^\dagger_{k,A}\ \hat{c}^\dagger_{k,B}\right]\left[\hat{\mathcal{H}}(k,t)\right]\begin{bmatrix}\hat{c}_{k,A}\\ \hat{c}_{k,B}\end{bmatrix} \tag{3.6}$$

where, for each $k \in$ BZ, the Hamiltonian $\hat{\mathcal{H}}(k,t)$ is a 2×2 Hermitean matrix, which one can always parameterize, in terms of the identity $\mathbb{1}$ and the three Pauli matrices $\hat{\boldsymbol{\sigma}}$. Here, as the trace of the matrix is zero, we can write $\hat{\mathcal{H}}(k,t) = \mathbf{R}(k,t)\cdot\hat{\boldsymbol{\sigma}}$, or, more explicitly:

$$\hat{\mathcal{H}}(k,t) = \begin{bmatrix} R_z & R_x - iR_y \\ R_x + iR + y & -R_z \end{bmatrix} = R_x(k,t)\hat{\sigma}_x + R_y(k,t)\hat{\sigma}_y + R_z(k,t)\hat{\sigma}_z\ . \tag{3.7}$$

A simple calculation [1] shows that:

$$\begin{aligned} R_x(k,t) &= -J_1(t) - J_2(t)\cos ka \\ R_y(k,t) &= -J_2(t)\sin ka \\ R_z(k,t) &= \Delta(t)\ , \end{aligned} \tag{3.8}$$

Notice that $\mathbf{R}(k+2\pi/a,t) = \mathbf{R}(k,t)$ and $\mathbf{R}(k,t+T) = \mathbf{R}(k,t)$, i.e., the effective magnetic field acting on the *pseudo-spin*-1/2 sublattice A/B degree-of-freedom is doubly periodic both in the BZ, and in time. Interestingly, the projection of $\mathbf{R}$ on the $x-y$ plane is simply a circumference of radius J_2 centered at $(-J_1, 0)$. Hence, you immediately realize that there are three possible situations:

1) $J_1 > J_2$: the circumference stays to the left of the origin, without enclosing it.

2) $J_1 < J_2$: the circumference encloses the origin.

3) $J_1 = J_2$: the circumference touches the origin.

Case 1) and 2) are realized, here, for $\varphi = 0$ and $\varphi = \pi$, where $R_z = \Delta = 0$ and hence the two circumferences are precisely on the $x-y$ plane; Case 3) is realized for $\varphi = \pi/2, 3\pi/2$, which are associated to $R_z = \Delta = \pm\Delta_0$. The "topological features" of case 1) and 2) above are very different: in the first case the magnetic field does not *wind* around the origin, while in the second case it does so. We will see the consequence of this fact when discussing edge states for the system with open boundary conditions.

Diagonalizing $\hat{\mathcal{H}}(k,t)$ for any given $k \in$ BZ at a fixed value of t is a simple spin-1/2 problem. The two eigenvalues are

$$\epsilon_{k,\pm}(t) = \pm|\mathbf{R}(k,t)| = \pm\sqrt{J_1^2 + J_2^2 + 2J_1J_2\cos ka + \Delta^2}\ . \tag{3.9}$$

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. 2.3). Let us denote by $|u_{k\pm}(t)\rangle$ the spinors corresponding to the two bands. Notice that we can parameterize them by simply knowing the angles $\theta_k(t)$ and $\phi_k(t)$ that the "magnetic field" $\mathbf{R}(k,t)$ 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 available orbitals $2N$, i.e., $N_e = N$. The crucial point (we will see this, with illustrations, later on, don't worry) will be *if*, when k spans over the BZ of the lattice and $t \in [0,T]$ (a torus, due to the double periodicity of $\mathbf{R}(k,t)$), this "magnetic field" $\mathbf{R}(k,t)$ will *wrap around the origin* of the Bloch sphere in spin-space or not. In the second case, we will see that there is no pumped charge; in the first case, there is. More about this, in a short while.

[1] Simply notice that:

$$\frac{J_1}{N}\sum_j\sum_{k,k'}^{\rm BZ}\left[\mathrm{e}^{-ikaj}\mathrm{e}^{ik'aj}\hat{c}^\dagger_{k,B}\hat{c}_{k,A} + \text{H.c.}\right] = J_1\sum_k^{\rm BZ}\left[\hat{c}^\dagger_{k,B}\hat{c}_{k,A} + \text{H.c.}\right]\ ,$$

and similarly for the other two terms.

3.2. The pumped charge

In the Rice-Mele model, working with PBC, there are two bands, a lower band $\epsilon_{k,-}(t)$ and an upper band $\epsilon_{k,+}(t)$ separated by a finite gap provided $|\mathbf{R}| \neq 0$. The condition $|\mathbf{R}| = 0$, as one can simply verify, implies the gapless metallic situation $J_1 = J_2 = J_0$ and $\Delta = 0$, which is never encountered during the dynamics. The dynamics can indeed be pictured in a two-dimensional plane, with $J_1 - J_2$ in the x-axis and Δ in the y-axis, as an ellipse wrapping around the dangerous gapless point $(J_1 - J_2 = 0, \Delta = 0)$. 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 $\epsilon_{k,-}(t)$ is fully occupied. For electrons on the continuum the associated $|u_{k,-}(t)\rangle$ would be a function $u_{k,-}(x,t)$ periodic over the unit cell of the crystal, but here we are working in tight-binding and $|u_{k,-}(t)\rangle$ is simply a two-component "spinor" telling us 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 $|u_{k,-}\rangle$ constitute a completely filled band, while $|u_{k,+}\rangle$ is an empty band. Hence, the charge pumped in a period becomes:

$$Q \;=\; -\int_0^T \mathrm{d}t \int_0^{\frac{2\pi}{a}} \frac{\mathrm{d}k}{2\pi}\, i\Big[\langle \partial_k u_{k,-}|\partial_t u_{k,-}\rangle - \langle \partial_t u_{k,-}|\partial_k u_{k,-}\rangle\Big] \,. \tag{3.10}$$

The object we have obtained looks like an antisymmetric form closely reminiscent of a Berry curvature integrated over the whole BZ and over time. We will see soon that indeed it is a Berry curvature for a spin-1/2 problem, *pulled back* into (k,t)-space by the (periodic) map $(k,t) \to \mathbf{R}(k,t)$ (more about this below).

The $|u_{k,-}\rangle$ appearing in Eq. (3.10) must be viewed as a composite function $|u_{k,-}(t)\rangle = |u_-(\mathbf{R}(k,t))\rangle$, 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:

$$\Big[\langle \partial_k u_{k,-}|\partial_t u_{k,-}\rangle - \langle \partial_t u_{k,-}|\partial_k u_{k,-}\rangle\Big] = \sum_{ij} \langle \partial_{R_i} u_-(\mathbf{R}))|\partial_{R_j} u_-(\mathbf{R}))\rangle\Big|_{\mathbf{R}=\mathbf{R}(k,t)} J_{ij}(k,t) \,,$$

where the Jacobian

$$J_{ij}(k,t) = \det \begin{bmatrix} \partial_k R_i & \partial_t R_i \\ \partial_k R_j & \partial_t R_j \end{bmatrix}_{k,t} \,, \tag{3.11}$$

appears. But $J_{ij} = -J_{ji}$ and therefore you immediately deduce that:

$$i\Big[\langle \partial_k u_{k,-}|\partial_t u_{k,-}\rangle - \langle \partial_t u_{k,-}|\partial_k u_{k,-}\rangle\Big] = \sum_{i<j} \mathcal{B}_{ij}(\mathbf{R}(k,t))\; J_{ij}(k,t) \,,$$

in terms of the Berry curvature of a spin-1/2 problem:

$$\mathcal{B}_{ij}(\mathbf{R}) = i\left[\langle \partial_{R_i} u_-(\mathbf{R})|\partial_{R_j} u_-(\mathbf{R})\rangle - \langle \partial_{R_j} u_-(\mathbf{R})|\partial_{R_i} u_-(\mathbf{R})\rangle\right] \;=\; \epsilon^{ijk}\, \frac{R_k}{2|\mathbf{R}|^3} \,, \tag{3.12}$$

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 pumped charge for the Rice-Mele model can be finally expressed as:

$$Q = \underbrace{-\int_0^T \mathrm{d}t \int_0^{\frac{2\pi}{a}} \frac{\mathrm{d}k}{2\pi} \sum_{i<j} \mathcal{B}_{ij}(\mathbf{R}(k,t))\; J_{ij}(k,t)}_{c_1} \;=\; -c_1 \,. \tag{3.13}$$

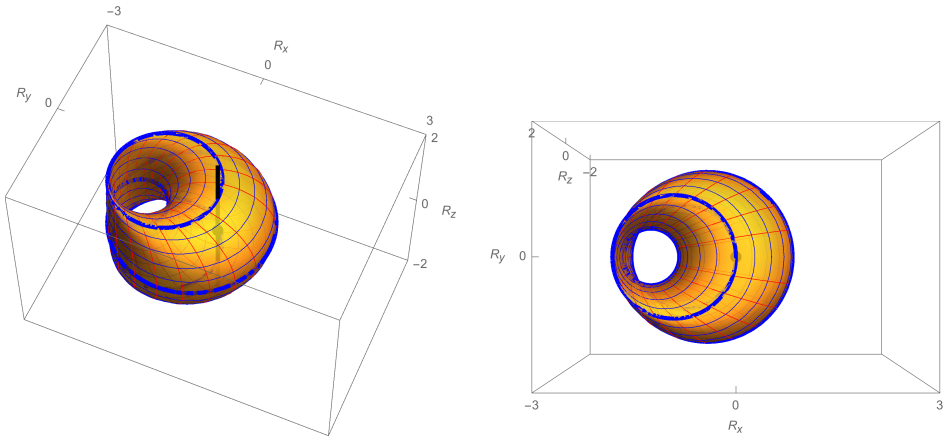

Figure 3.1.: Parametric plot of $\mathbf{R}(k,t)$ when k spans the BZ and t the period $[0,T]$. The surface has the topology of a torus: on the right, a top view of such torus.

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 $\mathbf{R}(k,t)$. You can explicitly write it as:

$$c_1 = \int_0^T \mathrm{d}t \int_0^{\frac{2\pi}{a}} \frac{\mathrm{d}k}{2\pi} \sum_{i<j} \mathcal{B}_{ij}(\mathbf{R}(\mathbf{k}))\, J_{ij}(\mathbf{k}) \;=\; \int_0^T \mathrm{d}t \int_0^{\frac{2\pi}{a}} \frac{\mathrm{d}k}{2\pi} \frac{\mathbf{R}}{|\mathbf{R}|^3} \cdot \left(\frac{\partial \mathbf{R}}{\partial k} \times \frac{\partial \mathbf{R}}{\partial t} \right) . \quad (3.14)$$

Notice that $\left(\frac{\partial \mathbf{R}}{\partial k} \times \frac{\partial \mathbf{R}}{\partial t}\right) \mathrm{d}k\mathrm{d}t$ is nothing but the "element of area" in the surface integral. What is really crucial is that this object is *topological* in nature, i.e., it must be an integer. Let us try to guess the result, guided by Gauss' law in electrostatic. Since the torus *encloses* the singularity at $\mathbf{R}^* = \mathbf{0}$, see Fig. 3.1, 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 $c_1 = \pm 1$. The *sign* that depends on how the surface $\mathbf{R}(k,t)$ is *oriented*, which, as you know, is important in calculating fluxes. The orientation is decided by $\left(\frac{\partial \mathbf{R}}{\partial k} \times \frac{\partial \mathbf{R}}{\partial t}\right)$, and points *outward* or *inward* depending on the direction in which we change the phase $\varphi(t)$: taking $\varphi(t) = -2\pi t/T$ would produce an opposite pumped charge.

It is perhaps worth summarizing the story, from the mathematical side, like this. You have the k-BZ and time-periodicity of the system, which already gives as a torus where (k,t) lives. Then you have a mapping $(k,t) \to \mathbf{R}(k,t)$ from the torus to $\mathbb{R}^3$, which defines a closed two-dimensional surface $\mathbf{R}(k,t)$ in $\mathbb{R}^3$: there is nothing particularly special or tricky about this mapping. But then, for each value of $\mathbf{R}(k,t)$ 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 — 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

$$(k,t) \to \mathbf{R} \to \hat{\mathbf{R}} = \frac{\mathbf{R}}{|\mathbf{R}|}$$

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 (k,t) runs over the BZ and the time-period, it must necessarily encounter a vortex singularity of the phase, otherwise not.

3.3. The Rice-Mele model with open boundaries: edge states

Until now we have worked with PBC and calculated the pumped charge as a bulk property. Let us see what happens if we imagine that the model is defined in a finite interval, i.e., open boundary conditions (OBC) are used. The Hamiltonian for a single particle can be regarded as a $2N \times 2N$ matrix of the form:

$$H(t) = \begin{pmatrix} \Delta & -J_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -J_1 & -\Delta & -J_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & -J_2 & \Delta & -J_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -J_1 & -\Delta & -J_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & -J_2 & \Delta & -J_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -J_1 & -\Delta & -J_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & -J_2 & \Delta & -J_1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -J_1 & -\Delta \end{pmatrix} . \tag{3.15}$$

Here we have shown it for $N = 4$, but the general form should be clear. Let us consider the cases in which $\Delta = 0$. There are two markedly different situations which we can consider: 1) $J_1 > J_2$ or 2) $J_1 < J_2$. To make the calculation extra simple, let us consider the two "extreme" representative cases 1) $J_2 = 0$ and 2) $J_1 = 0$. In the first case, the Hamiltonian is block-diagonal with 2×2 blocks of the form:

$$\begin{pmatrix} 0 & -J_1 \\ -J_1 & 0 \end{pmatrix}$$

whose eigenvalues are $\pm J_1$ with eigenfuntions being the two spinors of $\hat{\sigma}^x$: The ground state can be pictured as forming double-well dimers *inside the unit cell*, with the wave-function equally weighting the two orbitals in A and B. The spectrum is simple to picture: there are N eigenvalues $-J_1$ and N eigenvalues $+J_1$. In the second case, with $J_1 = 0$, the situation is similar but the double-well dimers are formed *across two unit cells*, as the relevant 2×2 blocks

$$\begin{pmatrix} 0 & -J_2 \\ -J_2 & 0 \end{pmatrix}$$

are now shifted with respect to the natural unit cell. Notably, sites $1A$ and NB are totally disconnected from those 2×2 blocks, hence *there are two eigenvalues which are* 0, sitting exactly in the middle of the gap formed by the remaining $N-1$ eigenvalues at $-J_2$ and $N-1$ eigenvalues at $+J_2$. The two 0-eigenvalues are associated to *edge states*: in the present extreme case, the wavefunctions are simply $(1, 0, \cdots, 0)$ (i.e., purely on the left edge) and $(0, \cdots, 0, 1)$ (i.e., purely on the right edge). If you consider a more realistic case where $J_2 > J_1 \neq 0$, then the two eigenvalues in the middle of the gap [2] persist, but the associated wavefunctions develop an exponential tail inside the bulk of the chain.

[2] Strictly speaking, the two eigenvalues are now split at $\pm\epsilon$, where ϵ is a quantity which is *exponentially small* in the length of the chain N.

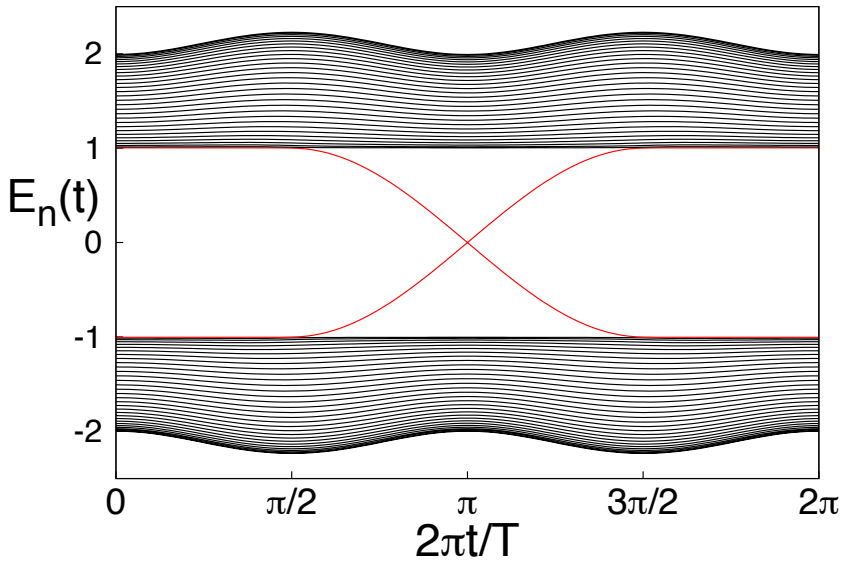

Figure 3.2.: Instantaneous eigenvalues for the Rice-Mele model with OBC. Here $N = 32$, $\delta_0 = J_0/2$ and $\Delta_0 = J_0$.

Fig. 3.2 illustrates the result of calculation of the spectrum of $H(t)$ as a function of t for $N = 32$. Notice that two central eigenvalues (indicated by the red curves) which *cross the spectral gap* as t increases from 0 to T. This situation is very commonly realized in *topological insulators*.

4. Floquet systems

In this chapter I will explain 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 $\hat{U}(t+n\tau,0) = \hat{U}(t,0)\hat{U}^n(\tau,0)$.

Hystorically, the Floquet theorem was derived in a completely classical context: the study of the stability of periodic orbits. If you want to know a bit more about the classical aspects of the story, read Appendix A. Here, before entering in the proof of the Floquet theorem, I want to start from a very simple classical problem that most of you have encountered before: the periodically driven pendulum.

4.1. Periodically driven pendulum

To be definite, let us start considering a very familiar one-dimensional system: the simple planar pendulum. If $q = \theta$ denotes the angle formed with the vertical, and $p_\theta = ml^2\dot{\theta}$ the associated momentum (indeed, an angular momentum), the Hamiltonian reads [1]

$$H(\theta, p_\theta) = \frac{p_\theta^2}{2ml^2} + mgl(1-\cos\theta) \, .$$

Here the phase-space is $n = 2$-dimensional. Different phase-trajectories associated to different E do not cross (uniqueness of the initial value problem in phase-space). [2] For $E < 2mgl$ the phase-trajectories are closed curves around the origin, while for $E > 2mgl$ they are unbound. $E = 2mgl$ is a *separatrix* between bounded and unbound orbits. It is simple to show that every bounded phase-trajectory for $n = 2$ must be associated to a *periodic motion*. This is very

[1] The Lagrangian is $L(\theta,\dot{\theta}) = ml^2\dot{\theta}^2/2 - mgl(1-\cos\theta)$, with a choice of the lowest position of the pendulum as a zero of potential energy. The associated momentum is therefore $p = \partial L/\partial\dot{\theta} = ml^2\dot{\theta}$.

[2] Different trajctories obviously cross in configuration space, which shows why the use of phase-space is advantageous.

simple to understand: starting from a point in phase space, the system moves, as t increases, along energy-countours (in a clockwise way) until, if the contour is a closed, returning (after a certain time T) to the initial point, and the motion repeats itself periodically. Indeed, you can show that every one-dimensional system (i.e., $n = 2$) with a conserved energy E can be fully integrated. [3]

So, in order to have chaos we must either leave $n = 2$ and go to higher dimensions (for instance a double pendulum, $n = 4$, or a non-Hamiltonian system with $n = 3$, there are many such models), or else you need a *driven* one-dimensional system, where energy is no longer conserved (time plays, in some way, the role of an effective extra dimension). Non-linearities have to be retained, however. Indeed, at the level of a linear system (i.e, a general quadratic Lagrangean/Hamiltonian) you know that you can always (at least in principle) diagonalize the problem by reducing to a system of independent *normal modes*, i.e., one-dimensional harmonic oscillators, each of which conserves its own energy, and can therefore be integrated. [4]

But let us return to our simple pendulum. The simplest system displaying chaos is indeed a periodically driven pendulum. Imagine you move the point of suspension O of the pendulum

[3] Let us see this in the usual Newtonian framework. From the conservation of $E = m\dot{x}^2/2 + V(x)$ we can deduce:

$$\dot{x} = \pm\sqrt{2(E - V(x))/m}\,,$$

where the $\pm$ sign is associated to the two possible directions of velocity. This first-order differential equation can be solved by separation of variables. If x_- and x_+ denote the two classical inversion points and we consider the trajectory moving to the right, starting at x_- at time t_- and ending at x_+ at time t_+, we have:

$$\int_{x_-}^{x_+} dx\, \frac{1}{\sqrt{2(E - V(x))/m}} = \int_{t_-}^{t_+} dt = (t_+ - t_-) = \frac{T}{2}\,,$$

where T indicates the period (the time to go forth to x_+ and back to x_-). The problem is (implicitly) solved "up to calculating integrals" (this is the meaning of "reducing to a quadrature", often used). Indeed, if you want $x(t)$ for t in the first half-period you simply need to calculate:

$$\int_{x_-}^{x(t)} dx\, \frac{1}{\sqrt{2(E - V(x))/m}} = t - t_-\,.$$

[4] For an harmonic system you can write the potential as $V = (1/2)\mathbf{u}^t \cdot \mathbf{K} \cdot \mathbf{u}$, i.e., a positive definite quadratic form (you can even allow for disorder in the spring constants). The equations of motions would then be $\mathbf{M}\ddot{\mathbf{u}} = -\mathbf{K} \cdot \mathbf{u}$, with $\mathbf{M} = \mathrm{diag}(M_1, \cdots, M_L)$. Rescaling by the square root of the masses brings the equations in the form $\ddot{\mathbf{x}} = -\left(\mathbf{M}^{-1/2} \cdot \mathbf{K} \cdot \mathbf{M}^{-1/2}\right) \cdot \mathbf{x} = -\tilde{\mathbf{K}} \cdot \mathbf{x}$, where $\mathbf{M}^{-1/2} = \mathrm{diag}(M_1^{-1/2}, \cdots, M_L^{-1/2})$. It is very simple, then, to show that $\tilde{\mathbf{K}} = \mathbf{M}^{-1/2} \cdot \mathbf{K} \cdot \mathbf{M}^{-1/2}$ is also *positive definite*. Diagonalize the matrix $\tilde{\mathbf{K}}$ and define the normal modes (eigenvectors) in terms of which the Hamiltonian becomes a sum of independent harmonic oscillators. There are special systems that remain integrable even for $n > 2$ in presence of non-linearities: these systems, essentially, have n conserved quantities (integrals of motions, the energy and $n-1$ other quantities) and can be reduced, by appropriate canonical transformations to simple decoupled one-dimensional Hamiltonians (a bit like the normal modes of the harmonic oscillator, with the only difference that the frequency ω_α of the simple motion in each two-dimensional phase-space depends on the value of the conserved quantity (energy, or better, action), while the ω_α of the harmonic normal modes is independent of the amplitude of the oscillations). A detailed account of these integrable Hamiltonian systems in given in the book by José and Saletan [9]. Indeed, a remarkable (and quite complicated) theorem in the theory of Hamiltonian systems states that even small perturbations around integrable Hamiltonians do not immediately make the system chaotic (KAM theorem): the most incommensurate integrable trajectories resist to perturbations for a while, and only a finite suitably large perturbation will lead to a truly chaotic behaviour.

in some periodic way, $y_O = A\cos 2\nu t$ (the reason for putting the factor 2 in the frequency will be clear in a moment). You can still use the Lagrangean formalism to derive the equation of motion, but you can also use the *equivalence principle*: formulated with a slightly pre-Einstein view-point, in the (non-intertial) frame in which the point of suspention is at rest, the system is subject to an extra fictitious acceleration $\ddot{y}_O = -4\nu^2 A\cos(2\nu t)$, and effectively this modifies the acceleration of gravity form g_0 to a $g(t) = g_0 - 4\nu^2 A\cos(2\nu t)$. The Hamilton's equations $\dot{\theta} = p_\theta/(ml^2)$ and $\dot{p}_\theta = -mlg(t)\sin\theta$ will then lead to

$$\frac{d^2\theta}{dt^2} = -\left[\omega^2 - \frac{4\nu^2 A}{l}\cos(2\nu t)\right]\sin\theta\ , \tag{4.1}$$

where $\omega = \sqrt{g_0/l}$ is the frequency of the unperturbed pendulum in the linear regime. This time-dependent non-linear equation needs to be studied numerically, in general, and displays chaos in certain regions of phase space. To proceed, one might think of exploring the region of validity of the linear regime at small θ, by studying the stability of the linear-equation solutions. Linearizing the equation, $\sin\theta \approx \theta$, we get:

$$\frac{d^2\theta}{dt^2} + \left[\omega^2 - \frac{4\nu^2 A}{l}\cos(2\nu t)\right]\theta = 0\ . \tag{4.2}$$

Now, let us make the equation dimensionless by measuring time in units of $1/\nu$, i.e., defining a dimensionless time $t' = \nu t$. Omitting for simplicity the prime, the equation in dimensionless form becomes:

$$\ddot{\theta} + [\epsilon - 2h\cos(2t)]\,\theta = 0\ . \tag{4.3}$$

where we have introduced the parameter $2h = 4A/l$, and $\epsilon = (\omega/\nu)^2$. In this form, it is known as Mathieu's equation.

Mathieu's equation

This equation should have a familiar look: it closely reminds of a well-known condensed matter textbook problem: the Schrödinger equation for particle in a one-dimensional periodic crystal potential of the form $V\cos(2qx)$, where $q = \pi/a$ is the Brillouin-zone (BZ) boundary in one-dimension (a is the periodicity of the lattice). Indeed, the Schrödinger equation for the stationary states of energy E will read:

$$\frac{d^2\psi}{dx^2} + \left[\frac{2mE}{\hbar^2} - \frac{2mV}{\hbar^2}\cos(2qx)\right]\psi(x) = 0\ . \tag{4.4}$$

To pass to a dimensionless form, let us measure lengths in units of $1/q = a/\pi$, i.e., define $x' = qx$. Again, omitting the prime we get:

$$\psi''(x) + \left[\frac{2mE}{(\hbar q)^2} - \frac{2mV}{(\hbar q)^2}\cos(2x)\right]\psi(x) = 0\ . \tag{4.5}$$

which clearly resembles the Mathieu equation for the linearized driven pendulum with the substitutions $t \to x$, $\theta(t) \to \psi(x)$, $(\omega/\nu)^2 \to 2mE/(\hbar q)^2$, and $2h \to 2mV/(\hbar q)^2$. One important aspect of this resemblance has to do with boundary conditions: the solutions to such periodic linear differential equations are themselves *not* strictly periodic, but only periodic "up-to-a-phase". In the Schrödinger case, this amounts to the familiar Bloch theorem: solutions $\psi_k(x)$, with energy E_k, can be written as $\psi_k(x) = e^{ikx}u_k(x)$ where k is a quasi-momentum and $u_k(x)$ is a periodic function: in the old dimensionful form, $u_k(x+a) = u_k(x)$. k can either run over all real axis (extended zone scheme) or be restricted to the first BZ,

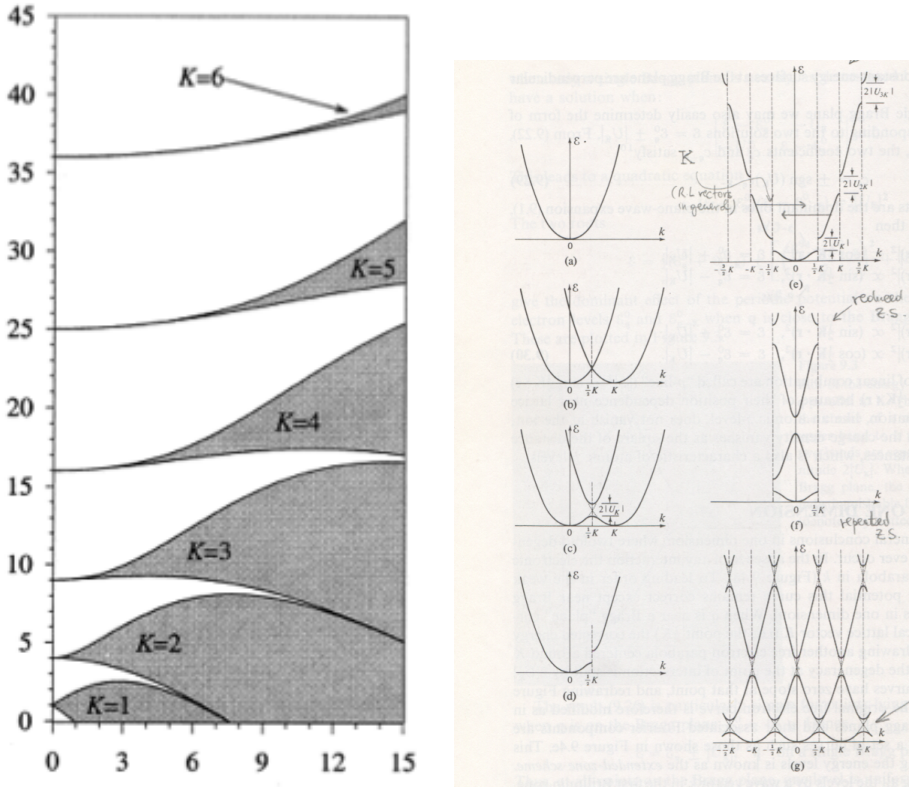

Figure 4.1.: Left: stability diagram for the Mathieu equation; in the y-axis you have $(\omega/\nu)^2$, in the x-axis the perturbation h. Shaded regions are (Lyapunov) unstable for the linear equation, and the full non-linear equation has to be studied. Right: Usual diagram for opening of gaps in the free-electron dispersion, taken from Ashkroft & Mermin. In the Bloch case solutions inside the spectral gaps are simply discarded because they are not associated to allowed wavefunctions.

at the price of introducing an extra band-index n, writing $\psi_{n,k}(x) = e^{ikx}u_{n,k}(x)$, and $E_{n,k}$. Notice that, for $V \neq 0$ the energies $E_{n,k}$ show *spectral gaps* Δ_n at the boundaries of the BZ, $k = \pm\pi/a = \pm q$, and at the BZ center $k = 0$, and this happens for all the bands, although the gaps rapidly decrease for increasing n. The lowest gap, obtained from degenerate first-order perturbation theory between the two degenerate solutions $e^{\pm iqx}$, coupled by the perturbation, is linear in $|V|$, while higher gaps are smaller because they come from higher order perturbations. The corresponding picture for the Mathieu's equation is, clearly, identical. By spanning the natural frequency ω^2 one encounters spectral gaps around the unperturbed boundary and Zone-center points, which happen to be at $(\omega/\nu)^2 = n^2$ with $n = 1, 2, \cdots$. Notice that ν is *half* the frequency of the perturbing field, and therefore the first instability is actually a *subharmonic* instability. The solutions can be written as

$$\theta_{n,\mu}(t) = e^{i\mu t}u_{n,\mu}(t) \,, \tag{4.6}$$

where n is a band index, $\mu \in [-\nu, \nu]$ is called Floquet quasi-energy, and $u_{n,\mu}(t)$ is a periodic function, with period $\tau = 2\pi/(2\nu) = \pi/\nu$. In this form, this results is known as *Floquet theorem.* [5]

[5] A word of caution is in order here. You should not think that the Schrödinger problem in Eq. (4.4) is the

4.2. 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:

$$i\dot{\boldsymbol{\psi}}(t) = \mathbf{H}(t) \cdot \boldsymbol{\psi}(t) \ , \tag{4.9}$$

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. [6] Take now, as initial value states, a complete 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. (4.9) starting from such a basis of initial values into a "matrix" $\boldsymbol{\Psi}(t)$ which will obviously satisfy:

$$i\dot{\boldsymbol{\Psi}}(t) = \mathbf{H}(t) \cdot \boldsymbol{\Psi}(t) \ , \tag{4.10}$$

with initial condition $\boldsymbol{\Psi}(0) = \boldsymbol{\Psi}_0$. [7] 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:

$$\boldsymbol{\Psi}(t) = \mathbf{U}(t, 0) \cdot \boldsymbol{\Psi}_0 \ , \tag{4.11}$$

---

quantum problem that correspond to the classical Mathieu's pendulum: they are just the same problem, with different names for the variables. The classical-quantum correspondence is, at the level of the full non-linear problems, that between the $H(t)$ of the classical driven pendulum

$$H_{\text{C driven pend.}}(\theta, p_\theta, t) = \frac{p_\theta^2}{2ml^2} + mlg(t)(1 - \cos\theta) \ , \tag{4.7}$$

where $g(t) = g_0 - 2hl\cos(2\nu t)$, and the corresponding equation for the quantum operator $\hat{H}$:

$$\hat{H}_{\text{Q driven pend.}}(t) = \frac{\hat{p}_\theta^2}{2ml^2} + mlg(t)(1 - \cos\theta) \ , \tag{4.8}$$

where now $\hat{p}_\theta$ is the quantum operator conjugate to θ, i.e., the angular momentum:

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

The appropriate Hilbert space is that of normalizable periodic functions $\psi(\theta)$, such that $\psi(\theta + 2\pi) = \psi(\theta)$. The eigenfunctions of angular momentum are $\phi_n(\theta) = e^{in\theta}/\sqrt{2\pi}$, but the cosine term couples them. The classical driven pendulum, being a non-linear dynamical system, must be dealt with an explicit integration of the classical Hamilton's equations. Quantum mechanically, on the contrary, we have a bonus: we can study the time-evolution through a Floquet approach by studying the evolution operator over just one period, but the price to pay is that we have an infinite-dimensional problem that we need to integrate over a period: some form of discretization/truncation is essential.

[6] 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.

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

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 $\mathbf{\Phi}(t) = \mathbf{\Psi}(t+\tau)$. It is a simple matter to prove that $\mathbf{\Phi}(t)$ obeys exactly the same SE in Eq. (4.10):

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

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 $\mathbf{\Phi}(t)$ obeys the same equation as $\mathbf{\Psi}(t)$, then there must exsist some other initial value $\mathbf{\Psi}'_0$ such that $\mathbf{\Phi}(t) = \mathbf{U}(t,0)\cdot\mathbf{\Psi}'_0$. 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 $\mathbf{\Phi}(0) = \mathbf{\Psi}(\tau)$ and that $\mathbf{U}(0,0) = \mathbb{1}$ we immediately deduce that $\mathbf{\Psi}'_0 = \mathbf{\Psi}(\tau)$. Therefore, we have just deduced that: $\mathbf{\Psi}(t+\tau) = \mathbf{U}(t,0)\cdot\mathbf{\Psi}(\tau) = \mathbf{U}(t,0)\cdot\mathbf{U}(\tau,0)\cdot\mathbf{\Psi}_0$, which, together with the always valid relationship $\mathbf{\Psi}(t+\tau) = \mathbf{U}(t+\tau,0)\cdot\mathbf{\Psi}_0$, implies the following identity:

$$\mathbf{U}(t+\tau,0) = \mathbf{U}(t,0)\cdot\mathbf{U}(\tau,0)\ . \tag{4.12}$$

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. [8] The proof now goes on along lines which you can easily anticipate. Consider $\mathbf{\Phi}(t) = \mathbf{\Psi}(t+n\tau)$ and again prove that is satisfies the same SE as $\mathbf{\Psi}(t)$, 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:

$$\mathbf{U}(t+n\tau,0) = \mathbf{U}(t,0)\cdot[\mathbf{U}(\tau,0)]^n\ . \tag{4.13}$$

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, and t is the residual time within the $(n+1)$-th period. The practical value of Eq. (4.13) 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 $t<\tau$. [9]

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. [10] 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: $\mathbf{\Psi}(\tau) = \mathbf{U}(\tau,0)\cdot\mathbf{\Psi}(0) =$

[8] 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*.

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

[10] 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.

$\mathbf{U}(\tau,0)$. Now, every unitary operator can be diagonalized by a unitary matrix. [11] Therefore, there must exist a complete set of states $\boldsymbol{\phi}_\alpha$ such that

$$\mathbf{U}(\tau,0)\cdot\boldsymbol{\phi}_\alpha = \lambda_\alpha\boldsymbol{\phi}_\alpha = e^{-i\mu_\alpha\tau}\boldsymbol{\phi}_\alpha\ , \tag{4.14}$$

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 $\boldsymbol{\Phi}$ we can rewrite the eigenvalue problem as:

$$\mathbf{U}(\tau,0)\cdot\boldsymbol{\Phi} = \boldsymbol{\Phi}\cdot e^{-i\boldsymbol{\mu}\tau} \qquad \Longrightarrow \qquad \mathbf{U}(\tau,0) = \boldsymbol{\Phi}\cdot e^{-i\boldsymbol{\mu}\tau}\cdot\boldsymbol{\Phi}^\dagger\ . \tag{4.15}$$

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 $\boldsymbol{\Phi}$: if you put it to the left, it does not work! The $\boldsymbol{\Phi}$ 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 $\boldsymbol{\Phi}$) and *Floquet quasi-energies* (the $\boldsymbol{\mu}$). And now comes the final piece of the story. Look again at the eigenvalue problem defining $\boldsymbol{\Phi}$, $\mathbf{U}(\tau,0)\cdot\boldsymbol{\Phi} = \boldsymbol{\Phi}\cdot e^{-i\boldsymbol{\mu}\tau}$: it tells us that, by evolving over a full period τ, the states $\boldsymbol{\Phi}$ get multiplied by a phase factor $e^{-i\boldsymbol{\mu}\tau}$. Consider now $\mathbf{U}(t,0)\cdot\boldsymbol{\Phi}$ for $t\le\tau$. By a seemingly trivial manipulation, write it as:

$$\mathbf{U}(t,0)\cdot\boldsymbol{\Phi} = \underbrace{\mathbf{U}(t,0)\cdot\boldsymbol{\Phi}\cdot e^{+i\boldsymbol{\mu}t}}_{\boldsymbol{\Phi}(t)}\cdot e^{-i\boldsymbol{\mu}t} = \boldsymbol{\Phi}(t)\cdot e^{-i\boldsymbol{\mu}t}\ , \tag{4.16}$$

where the newly defined quantity

$$\boldsymbol{\Phi}(t) \stackrel{def}{=} \mathbf{U}(t,0)\cdot\boldsymbol{\Phi}\cdot e^{+i\boldsymbol{\mu}t}\ , \tag{4.17}$$

is time-periodic because $\boldsymbol{\Phi}(\tau) = \boldsymbol{\Phi}(0) = \boldsymbol{\Phi}$. Eq. (4.16) is the promised result: we have found a complete set of states $\boldsymbol{\Phi}$, the Floquet modes, which evolve with a time-periodic part $\boldsymbol{\Phi}(t)$ times a phase factor $e^{-i\boldsymbol{\mu}t}$. Equivalently, we can rewrite Eq. (4.17) in the form:

$$\mathbf{U}(t,0) = \boldsymbol{\Phi}(t)\cdot e^{-i\boldsymbol{\mu}t}\cdot\boldsymbol{\Phi}^\dagger(0)\ , \tag{4.18}$$

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

$$\mathbf{U}(t,t') = \boldsymbol{\Phi}(t)\cdot e^{-i\boldsymbol{\mu}(t-t')}\cdot\boldsymbol{\Phi}^\dagger(t')\ . \tag{4.19}$$

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 $\boldsymbol{\Phi}$ of $\mathbf{U}(\tau,0)$, and the corresponding eigenvalues phases $\boldsymbol{\mu}$, give us states which propagate as a periodic part $\boldsymbol{\Phi}(t)$ times a phase factor $e^{-i\boldsymbol{\mu}t}$. [12] A totally equivalent way of reformulating

[11] Indeed, any *normal* operator, i.e., such that $A^\dagger A = AA^\dagger$ 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.

[12] For those of you who cannot renounce to the Dirac notation, here is how Eq. (4.18) looks like with bras and kets:

$$\mathbf{U}(t,0) = \sum_\alpha e^{-i\mu_\alpha t}|\boldsymbol{\phi}_\alpha(t)\rangle\langle\boldsymbol{\phi}_\alpha(0)|\ . \tag{4.20}$$

the previous findings is the following: We can construct a complete set of solutions of the time-dependent SE

$$i\frac{d}{dt}\boldsymbol{\psi}_\alpha(t) = \mathbf{H}(t)\cdot\boldsymbol{\psi}_\alpha(t)\ ,$$

which has the following form:

$$\boldsymbol{\psi}_\alpha(t) = \mathrm{e}^{-i\mu_\alpha t}\boldsymbol{\phi}_\alpha(t)\ ,$$

where $\boldsymbol{\phi}_\alpha(t+\tau) = \boldsymbol{\phi}_\alpha(t)$ is *periodic*. Evidently, the various $\boldsymbol{\phi}_\alpha(t)$ are simply the "columns" of the unitary $\boldsymbol{\Phi}(t)$. In this last form, the similarity with Bloch theorem in solid state is quite transparent.

4.3. Dynamical localization

4.3.1. 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:

$$g(t) = g\ \delta_P(t/\tau) \stackrel{def}{=} g\sum_n \delta(t/\tau - n) = g\tau\sum_n \delta(t-n\tau)\ , \tag{4.21}$$

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 $\int_{t_0}^{t_0+\Delta t} dtF(t) = I$ 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:

$$H_{\mathrm{kp}}(\theta, p_\theta, t) = \frac{p_\theta^2}{2ml^2} - mlg\ \delta_P(t/\tau)\cos\theta\ . \tag{4.22}$$

from which the following Hamilton's equations follow immediately:

$$\begin{aligned} \dot{\theta} &= \frac{p_\theta}{ml^2} \\ \dot{p}_\theta &= -mlg\ \delta_P(t/\tau)\sin\theta\ . \end{aligned} \tag{4.23}$$

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:

$$\begin{aligned} \theta_{n+1} - \theta_n &= \frac{p_n^+}{ml^2}\tau \\ p_n^+ - p_n^- &= -mlg\tau \sin\theta_n \ . \end{aligned} \tag{4.24}$$

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

$$\begin{aligned} \theta_{n+1} &= \theta_n + L_{n+1} \\ L_{n+1} &= L_n - K\sin\theta_n \ , \end{aligned} \tag{4.25}$$

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. (4.25) defines a *discrete map* in phase space (θ, p_θ), known as *standard map*, or Chirikov map. Formally, we have:

$$(\theta_{n+1}, L_{n+1}) = Z_K(\theta_n, L_n) \ . \tag{4.26}$$

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. [13] 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. 4.2. To fix the ideas, suppose you have the non-interacting map with $K = 0$ (no kicks): Z_0. This simply gives:

$$\begin{aligned} \theta_{n+1} &= \theta_n + L_{n+1} \\ L_{n+1} &= L_n \ , \end{aligned} \tag{4.27}$$

[13] 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 [9], 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. 4.2 (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 [9]. 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:

$$\begin{aligned} L_1 &= -K \sin\theta_0 && \longrightarrow \theta_1 = \theta_0 + L_1 \\ L_2 &= -K \sin\theta_0 - K \sin\theta_1 && \longrightarrow \theta_2 = \theta_1 + L_2 \\ &\cdots \\ L_n &= -K \textstyle\sum_{j=0}^{n-1} \sin\theta_i \end{aligned} \tag{4.28}$$

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

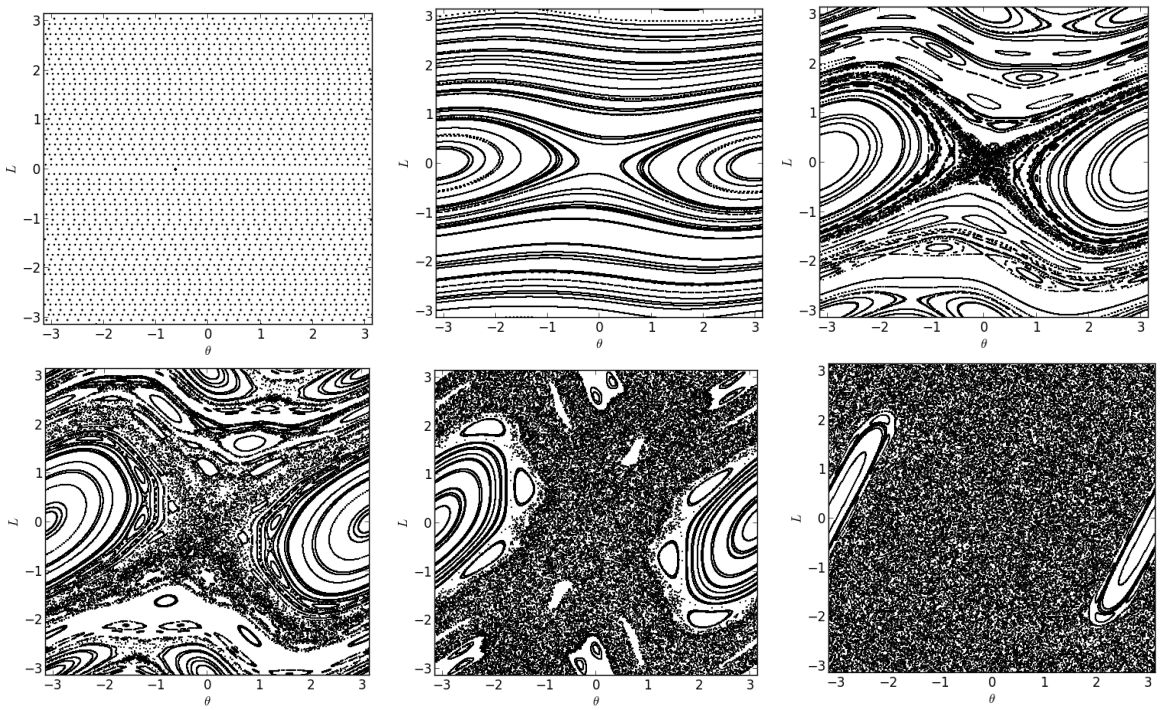

Figure 4.2.: Standard map iterations for increasing values of k (from top left to bottom right): $K = 0, 0.25, 0.75, 1, 1.5, 4$. For each K, the initial values of L_0 where 62 equispaced points in $[-\pi, \pi)$, while the corresponding initial values of θ_0 where selected randomly in $[\pi, \pi)$. The 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:

$$\langle L_n^2 \rangle = \langle K^2 \sum_{j=0}^{n-1} \sum_{j'=0}^{n-1} \sin\theta_j \sin\theta_{j'} \rangle \approx K^2 \sum_{j=0}^{n-1} \langle \sin^2\theta_j \rangle \approx \frac{K^2}{2} n = Dn \ , \tag{4.29}$$

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 $L_0 = 0$:

$$\begin{aligned} f_n(L) &= \langle \delta(L - L_n) \rangle = \langle \int_{-\infty}^{+\infty} \frac{dt}{2\pi} \, e^{it(L-L_n)} \rangle = \langle \int_{-\infty}^{+\infty} \frac{dt}{2\pi} \, e^{itL} \prod_{j=0}^{n-1} e^{iKt\sin\theta_j} \rangle \\ &\approx \int_{-\infty}^{+\infty} \frac{dt}{2\pi} \, e^{itL} \prod_{j=0}^{n-1} \langle e^{iKt\sin\theta_j} \rangle \approx \int_{-\infty}^{+\infty} \frac{dt}{2\pi} \, e^{itL} [J_0(Kt)]^n \\ &\approx \int_{-\infty}^{+\infty} \frac{dt}{2\pi} \, e^{itL} e^{-nK^2t^2/4} = \frac{1}{\sqrt{\pi K^2 n}} e^{-L^2/(K^2 n)} \ . \end{aligned} \tag{4.30}$$

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.

4.3.2. The quantum kicked pendulum

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

$$\hat{H}_{\rm kp}(t) = \frac{\hat{p}_\theta^2}{2ml^2} - mlg \ \delta_P(t/\tau) \cos\theta \ , \tag{4.31}$$

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:

$$\hat{H}_{\rm p-kick}(t) = \hat{T} + \delta_P(t/\tau) \ \hat{V} \ , \tag{4.32}$$

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:

$$\mathbf{U}(\tau, 0) = \lim_{\Delta t \to 0} e^{-\frac{i}{\hbar}(\hat{T} + \frac{\tau}{\Delta t}\hat{V})\Delta t} e^{-\frac{i}{\hbar}\hat{T}(\tau - \Delta t)} = e^{-\frac{i}{\hbar}\hat{V}\tau} e^{-\frac{i}{\hbar}\hat{T}\tau} \ . \tag{4.33}$$

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:

$$\mathbf{U}(\tau, 0) = e^{ik\cos\theta} e^{-i\hat{L}^2 q} \ , \tag{4.34}$$

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

$$\begin{aligned} k &= \frac{ml^2\omega_0^2\tau}{\hbar} \\ q &= \frac{\hbar\tau}{2ml^2} \ . \end{aligned} \tag{4.35}$$

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

$$2kq = \omega_0^2\tau^2 = K \ , \tag{4.36}$$

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:

$$|\psi(n\tau)\rangle = \hat{U}^n |\psi(0)\rangle \ . \tag{4.37}$$

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 $+\infty$:

$$\langle\theta|m\rangle = \frac{1}{\sqrt{2\pi}} e^{im\theta} \ . \tag{4.38}$$

Inserting identities in the form

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

we easily arrive at:

$$\psi_m^{(n)} = \sum_{m'=-\infty}^{+\infty} [\hat{U}^n]_{mm'} \ \psi_{m'}^{(0)} \ , \tag{4.39}$$

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

$$P_n(m) = |\psi_m^{(n)}|^2 = \left| \sum_{m'=-\infty}^{+\infty} [\hat{U}^n]_{mm'} \psi_{m'}^{(0)} \right|^2 \ , \tag{4.40}$$

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:

$$\langle\hat{L}^2\rangle_n = \langle\psi(n\tau)|\hat{L}^2|\psi(n\tau)\rangle = \sum_{m=-\infty}^{+\infty} m^2 P_n(m) \ . \tag{4.41}$$

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

$$[\hat{U}]_{mm'} = \langle m|e^{ik\cos\theta}e^{-i\hat{L}^2 q}|m'\rangle = e^{-iq(m')^2} i^{m-m'} J_{m-m'}(k) \; , \tag{4.42}$$

where we have made use of the Bessel identity:

$$\int_0^{2\pi} \frac{d\theta}{2\pi}\, e^{ik\cos\theta} e^{im\theta} = i^m J_m(k) \; . \tag{4.43}$$

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 $e^{-i\mu_i\tau}$:

$$\hat{U}(\tau, 0) = \sum_i e^{-i\mu_i\tau} |\phi_i\rangle\langle\phi_i| \; , \tag{4.44}$$

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 $\hat{U}$:

$$\hat{U}^n = \sum_i e^{-in\mu_i\tau} |\phi_i\rangle\langle\phi_i| \; , \tag{4.45}$$

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

$$[\hat{U}^n]_{mm'} = \sum_i e^{-in\mu_i\tau} \langle m|\phi_i\rangle\langle\phi_i|m'\rangle = \sum_i e^{-in\mu_i\tau} [\Phi]_{mi}[\Phi^\dagger]_{im'} \; , \tag{4.46}$$

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:

$$P_n(m) = |\psi^{(n)}_m|^2 = \left| \sum_i e^{-in\mu_i\tau} \sum_{m'} [\Phi]_{mi}[\Phi^\dagger]_{im'} \psi^{(0)}_{m'} \right|^2 \; . \tag{4.47}$$

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. 4.47 can be done easily, obtaining:

$$P_n(m) = \left| \sum_i e^{-in\mu_i\tau} [\Phi]_{mi}[\Phi^\dagger]_{i0} \right|^2 \; . \tag{4.48}$$

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

$$P_{n=0}(m) = \left| \sum_i [\Phi]_{mi}[\Phi^\dagger]_{i0} \right|^2 = \left| [\Phi\Phi^\dagger]_{m0} \right|^2 = \delta_{m,0} \; , \tag{4.49}$$

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:

$$\left|\sum_i z_i\right|^2 = \sum_{i,j} z_i z_j^* = \sum_i |z_i|^2 + \sum_{i\neq j} z_i z_j^* \ . \tag{4.50}$$

In some sense, you could call the off-diagonal contributions *interference terms.* [14] If we apply this simple idea to the expression in Eq. 4.48 we end up splitting it as follows:

$$P_n(m) = \underbrace{\sum_i \left|[\Phi]_{mi}[\Phi^\dagger]_{i0}\right|^2}_{P^{\rm Diag}(m)} + \underbrace{\sum_{i\neq j} e^{-in(\mu_i-\mu_j)\tau}[\Phi]_{mi}[\Phi^\dagger]_{i0}[\Phi]^*_{mj}[\Phi^\dagger]^*_{j0}}_{P_n^{\rm Interf}(m)} \ . \tag{4.51}$$

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:

$$P^{\rm Diag}(m=0) = \sum_i \left|[\Phi]_{0i}[\Phi^\dagger]_{i0}\right|^2 = \sum_i \left||[\Phi]_{0i}|^2\right|^2 = \sum_i |[\Phi]_{0i}|^4 \leq 1 \ , \tag{4.52}$$

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:

$$P_n(m) = P^{\rm Diag}(m) + P_n^{\rm Interf}(m) \overset{n\to\infty}{\longrightarrow} P^{\rm Diag}(m) \ , \tag{4.53}$$

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.*

[14] 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. 4.48 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":

$$P^{\rm Diag}(m) \sim \frac{1}{l_s} e^{-2|m|/l_s} \ , \tag{4.54}$$

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:

$$\langle\theta|\hat{U}|\psi(0)\rangle\Big|_{q=2\pi} = e^{ik\cos\theta} e^{i2\pi\hat{L}^2} \psi^{(0)}(\theta) \ . \tag{4.55}$$

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:

$$\langle\theta|\hat{U}|\psi(0)\rangle\Big|_{q=2\pi} = e^{ik\cos\theta} \psi^{(0)}(\theta) \ . \tag{4.56}$$

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:

$$\psi^{(n)}(\theta) = \langle\theta|\hat{U}^n|\psi(0)\rangle\Big|_{q=2\pi} = e^{ink\cos\theta} \psi^{(0)}(\theta) \ , \tag{4.57}$$

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

$$\begin{aligned} \langle\hat{L}^2\rangle_n = \int_0^{2\pi} \left|\frac{\partial}{\partial\theta}\psi^{(n)}(\theta)\right|^2 &\overset{q=2\pi}{=} \int_0^{2\pi} \left|e^{ik\cos\theta}\frac{\partial}{\partial\theta}\psi^{(0)}(\theta) - ink\sin\theta e^{ink\cos\theta}\psi^{(0)}(\theta)\right|^2 \\ &\overset{q=2\pi}{=} \langle\hat{L}^2\rangle_0 + n^2k^2 \int_0^{2\pi} \sin^2\theta \left|\psi^{(0)}(\theta)\right|^2 + O(n) \ , \end{aligned} \tag{4.58}$$

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.

A. Sensitivity to initial conditions: Lyapunov exponents

Let $\mathbf{X}^{(0)}(t) = (\mathbf{x}^{(0)}(t), \mathbf{p}^{(0)}(t))$ collectively denote the solution of a Newtonian (Hamiltonian or dissipative, doesn't matter) flow starting from some initial condition at time t_0: $\mathbf{X}^{(0)}(t_0) = \mathbf{X}_0$. Consider now a different phase-trajectory $\mathbf{X}(t)$ starting at $t = t_0$ from a nearby point $\mathbf{X}_0 + \mathbf{w}_0$, and define $\mathbf{w}(t)$ to be the deviation $\mathbf{X}(t) - \mathbf{X}^{(0)}(t) = \mathbf{w}(t)$. In components, expanding the flow equation around the starting trajectory we have:

$$\dot{X}_i = \dot{X}_i^{(0)} + \dot{w}_i = F_i(\mathbf{X}^{(0)}(t) + \mathbf{w}(t), t) = F_i(\mathbf{X}^{(0)}(t), t) + \sum_j \frac{\partial F_i}{\partial X_j}(\mathbf{X}^{(0)}(t), t)\; w_j(t) + \cdots \;, \tag{A.1}$$

where the $\cdots$ indicate higher order terms in $\mathbf{w}$. Defining $\mathbf{J}(t)$ to be the Jacobian matrix

$$\mathbf{J}_{ij}(t) = \frac{\partial F_i}{\partial X_j}(\mathbf{X}^{(0)}(t), t) \;, \tag{A.2}$$

and dropping higher order terms we end-up with the linearized equations:

$$\dot{\mathbf{w}}(t) = \mathbf{J}(t) \cdot \mathbf{w}(t) \;. \tag{A.3}$$

If $\mathbf{J}$ was *independent of* t, then the solution of the linearized problem would be an exponential $\mathbf{w}(t) = e^{\mathbf{J}(t-t_0)} \cdot \mathbf{w}_0$, and we would analize the stability in terms of eigenvalues of $\mathbf{J}$ (stability is guaranteed if the real part of all eigenvalues is negative). Unfortunately, when $\mathbf{J}$ depends on t, the solution can only be given in terms of a "time-ordered exponential". Nevertheless, the fact that $\mathbf{w}(t)$ must be *linearly related* to $\mathbf{w}(t_0)$ is simple to grasp: the matrix connecting the two is the *propagator* $\mathbf{L}(t, t_0)$ in terms of which [1]

$$\mathbf{w}(t) = \mathbf{L}(t, t_0) \cdot \mathbf{w}(t_0) \;. \tag{A.4}$$

[1] Evidently, the propagator $\mathbf{L}(t, t_0)$ satisfies an entirely similar linear equation:

$$\frac{d}{dt}\mathbf{L}(t, t_0) = \mathbf{J}(t) \cdot \mathbf{L}(t, t_0) \;,$$

whose (formal) solution is:

$$\mathbf{L}(t, t_0) = \mathrm{Texp}[\int_{t_0}^{t} dt' \mathbf{J}(t')] \stackrel{def}{=} \sum_{n=0}^{\infty} \frac{1}{n!} \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_n \mathrm{T}[\mathbf{J}(t_1) \cdots \mathbf{J}(t_n)] \;,$$

where, by definition, $\mathrm{T}[\cdots]$ orders the operators with the prescription "later times to the left". Among the properties of the propagator, it is worth mentioning that

$$\mathbf{L}(t, t_0) = \mathbf{L}(t, t_1)\mathbf{L}(t_1, t_0)$$

The mathemathitians have been able to prove (within the theory of ergodic multiplicative processes) that the following limit exists:

$$\lambda_L = \lim_{t\to\infty} \frac{1}{2t} \log\left(\mathrm{Tr}[\mathbf{L}^\dagger(t,t_0)\mathbf{L}(t,t_0)] \right) . \tag{A.5}$$

λ_L is called the (maximum) Lyapunov exponent. Notice that in the time-independent case, this is just the maximum real part of the eigenvalues of $\mathbf{J}$. Whenever $\lambda_L > 0$, the solution $\mathbf{X}^{(0)}(t)$ is unstable and small deviations $\mathbf{w}_0$ of the initial condition are (generally) amplified in an exponential way. [2]

The previous theory generalizes to the time-dependent case the "small oscillation" expansion around equilibrium points which should be familiar to the reader.

Let us now consider the important case when the trajectory $\mathbf{X}^{(0)}(t)$ is *periodic* in time, $\mathbf{X}^{(0)}(t+\tau) = \mathbf{X}^{(0)}(t)$ (for instance, a "limiting cycle" in a dissipative system). Consider also, for simplicitiy, the case in which $\mathbf{F}(\mathbf{X})$ does not depend on time explicitly. Then, the linearized problem has a $\mathbf{J}(t)$ which is periodic: $\mathbf{J}(t+\tau) = \mathbf{J}(t)$. One should *not* think that a solution of the linear problem in Eq. (A.3) with a periodic $\mathbf{J}(t)$ should be periodic as well. If you are familiar with the elementary theory of electronic bands in a crystalline solid, recall that the solutions (the Bloch states $\psi_k(x)$) of the problem are themselves not periodic, but, as assured by Bloch's theorem, can be written as the product of a periodic function $u_k(x)$ times a phase factor e^{ikx}: $\psi_k(x) = e^{ikx}u_k(x)$. What we are going to show is, essentially, an identical result for the solutions of the periodic linear problem in Eq. (A.3). Indeed, a theory due to Floquet and Lyapunov (see for instance Gantmakher, *Theory of Matrices*) shows that a basis of solutions can always be written as a product of a time-periodic part $\mathbf{P}(t)$ times a pure "exponential term" $\mathbf{Y}(t) = e^{t\mathbf{R}}$:

$$\mathbf{W}(t) = \mathbf{P}(t) \cdot e^{t\mathbf{R}} .$$

Let us see how this comes about. *First*: a n-dimensional linear problem admits n linearly independent solutions. We can think of the $\mathbf{w}$ appearing in Eq. (A.3) to be a $n \times n$ matrix, by collecting together n linearly independent solutions as columns of a matrix $\mathbf{W}$, which we will refer to as a *matrix integral*. *Second*: if $\mathbf{W}(t)$ is a matrix integral of Eq. (A.3), then $\mathbf{W}(t+\tau)$ is also a matrix integral, as one can readily verify:

$$\frac{d}{dt}\mathbf{W}(t+\tau) = \mathbf{J}(t+\tau)\cdot\mathbf{W}(t+\tau) = \mathbf{J}(t)\cdot\mathbf{W}(t+\tau) , \tag{A.6}$$

by using the fact that $\mathbf{J}(t+\tau) = \mathbf{J}(t)$. *Third:* since $\mathbf{W}(t+\tau)$ and $\mathbf{W}(t)$ are both matrix integrals of the same equation, one must have that $\mathbf{W}(t) = \mathbf{L}(t,0)\cdot\mathbf{W}(0)$ and $\mathbf{W}(t+\tau) = \mathbf{L}(t,0)\cdot\tilde{\mathbf{W}}(0)$ with the same propagator $\mathbf{L}(t,0)$ but with different initial conditions $\mathbf{W}(0)$ and $\tilde{\mathbf{W}}(0)$. As a a simple consequence, one then derives that

$$\mathbf{W}(t+\tau) = \mathbf{W}(t)\cdot\mathbf{W}^{-1}(0)\cdot\tilde{\mathbf{W}}(0) = \mathbf{W}(t)\cdot\mathbf{L} , \tag{A.7}$$

where $\mathbf{L} = \mathbf{W}^{-1}(0)\cdot\tilde{\mathbf{W}}(0)$ is a non-singular transformation (independent of t, this is the crucial point) which shows that the $\mathbf{W}(t+\tau)$ are indeed linear combinations of the solutions

[2] Obviously, if the flow is Hamiltonian, since by Liouville's theorem the phase-space volume must be conserved, there must be "directions" that are exponentially shrinked, as $e^{-\lambda_L t}$.

$\mathbf{W}(t)$. To obtain $\mathbf{L}$, it is enough to focus on the matrix solution with initial conditions at time $t = 0$ given by the identity matrix: $\mathbf{W}(t = 0) = \mathbf{1}$. Then, by Eq. (A.7)

$$\mathbf{L} = \mathbf{W}(\tau) \tag{A.8}$$

$$\frac{d}{dt}\mathbf{W}(t) = \mathbf{J}(t) \cdot \mathbf{W}(t)$$

$$\mathbf{W}(t = 0) = \mathbf{1} \, . \tag{A.9}$$

In other words, $\mathbf{L}$ is simply the time-evolved, over one period, of the unit matrix, and therefore coincides with the propagator from 0 to τ:

$$\mathbf{L} = \mathbf{L}(\tau, 0) \, .$$

(This is the reason for using the same symbol for two quantities that, a priori, are not the same object!) [3] Exploiting $\mathbf{L}$, we can perform a *Lyapunov transformation* of the variables, which transforms the time-dependent problem in Eq. (A.3) into a time-independent linear problem. Indeed, let us extract a periodic part, by writing (in a slightly tautological way):

$$\mathbf{W}(t) = \mathbf{W}(t) \cdot e^{-(t/\tau)\ln \mathbf{L}} e^{(t/\tau)\ln \mathbf{L}} = \mathbf{P}(t) \cdot \mathbf{Y}(t) \tag{A.10}$$

where $\mathbf{Y}(t) = e^{(t/\tau)\ln \mathbf{L}}$ and

$$\mathbf{P}(t) = \mathbf{W}(t) \cdot e^{-(t/\tau)\ln \mathbf{L}} \, . \tag{A.11}$$

Evidently, $\mathbf{P}(t)$ is periodic, since $\mathbf{P}(0) = \mathbf{P}(\tau) = \mathbf{W}(0)$. (Notice that, by being careful with the order of the matrices, these relationships are true even if $\mathbf{W}(0)$ is not the identity.) Therefore, the *stability properties of the problem described by the* $\mathbf{W}$ *and that described by the* $\mathbf{Y}$ *are identical*! But, on the other hand, it is very simple to show that $\mathbf{Y}(t)$ verifies the following *time-independent* linear problem:

$$\frac{d}{dt}\mathbf{Y}(t) = \frac{1}{\tau} \ln \mathbf{L} \cdot \mathbf{Y}(t) \, , \tag{A.12}$$

whose solution, starting from the identity at $t = 0$, is indeed $\mathbf{Y}(t) = e^{(t/\tau)\ln \mathbf{L}}$. Therefore, in conclusion, all we have to do to study the stability of the problem in Eq. (A.3) is simply to study the stability of the problem in Eq. (A.12), which is relatively easy. If we call ν_i the (complex, in general) eigenvalues of $\mathbf{L}$, then the relevant eigenvalues of the time-independent linear problem in Eq. (A.12) are simply $\lambda_i = \tau^{-1} \ln \nu_i$, and stability requires that all λ_i have *negative real parts*, $\mathrm{Re}\lambda_i < 0$. In terms of the eigenvalues of $\mathbf{L}$, therefore, stability requires that $|\nu_i| < 1$.

[3] One remark is in order: from the propagator view-point one would conclude that $\mathbf{W}(t+\tau) = \mathbf{L}(t+\tau, t)\mathbf{W}(t)$, but one should not hurry up and deduce that $\mathbf{L}(t + \tau, t) = \mathbf{L}(\tau, 0) = \mathbf{L}$, a relationship which is *wrong*: if we want to relate the two matrix solutions by $\mathbf{L}$, then we have to put it to the *right* of $\mathbf{W}(t)$, not to the left. The reason is trivial: $W_{ij}(t + \tau) = \sum_k W_{ik}(\tau) L_{kj}$ means that I obtain the (new) solution 'j' at point 'i' by making linear combinations of all the (old) solutions 'k' at the same point 'i', with coefficients given by the matrix L_{kj}. What you can prove to be correct, instead, is that

$$\mathbf{L}(t + \tau, \tau) = \mathbf{L}(t, 0)$$

while in general

$$\mathbf{L}(t + \tau, t) = \mathbf{L}(t + \tau, \tau) \cdot \mathbf{L}(\tau, 0) \cdot \mathbf{L}(0, t) = \mathbf{L}(t, 0) \cdot \mathbf{L}(\tau, 0) \cdot \mathbf{L}^{-1}(t, 0) \, .$$

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