The Quantum Cluster Approach to Spin Liquid

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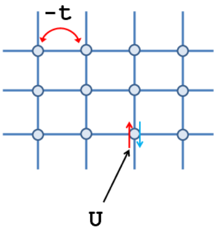
Outline of the talk I

Hubbard model

Graphical representation of the interaction of the Hubbard Model



The Hamiltonian of the Hubbard model is given by

$$H = -t \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + h.c. + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

HB continued....

With U=0, the Hubbard Hamiltonian can be diagonalized with the help of the Fourier Transform

$$H_0 = \sum_{k\sigma} (\epsilon(k) - \mu) c^\dagger_{k\sigma} c_{k\sigma}$$

$$\epsilon_k = -2t(cos(k_x) + cos(k_y))$$

This model has SU(2)xU(1) Global symmtery.

- at half-filling with increasing U, HB exhibits MIT at some critical value of U.
- In the Mott Phase the charge is gapped out and the only relevant DOF are spins.

In the mott phase the HB may be projected out to singly occupied space in the power of t/U, in the lowest order of t/U the effective hamiltonian is described by

$$H_h = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

- S_i spin operator which lives on the lattice sites. J exchange interaction.
- The Ground state of this Hamiltonian on the square lattice is AFM.
- On the frustated lattice spins may not organizzed in the long-range order.
- Possible to realize the phases where spins are in disordered state.
- such phases called the quantum spin liquid (QSL).

Spin Hamiltonians

Model Spin hamiltonians that were investigated to look for QSLs

- Heisenberg model on the Kagome Lattice
- Heisenberg model on triangular lattice
- Kitaev-Heisenberg model on the honeycomb lattice

$$H_h = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \qquad H_k = J \sum_{\langle ij \rangle^\alpha} S_i^\alpha S_j^\alpha$$

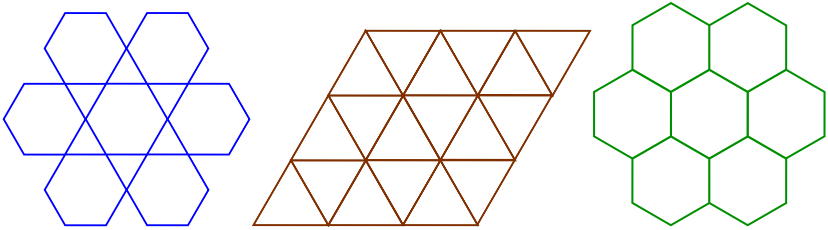
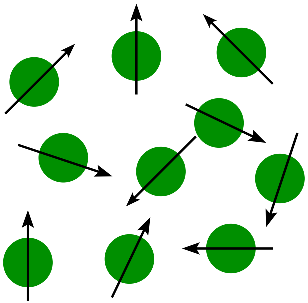


Figure: Kagome lattice, Triangular lattice and honeycomb lattice

Spin Liquids

- Exotic new phases of matter.
- Mott - insulating phases with no magnetic order down to lowest of temperatures.
- Disorder due to quantum fluctuations and frustration.



Many types of Spin Liquids depending on the symmetry properties of the phase

- Short range RVB spin liquid
- Algebraic spin liquid
- Chiral spin liquid
- U(1) spin Liquid

Types of Spin Liquid

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- SU(2) spin Liquid

Around 180 different types of QSLs exist in theory based on projective symmetri groups and quantum orders. (X. G. Wen Phys Rev B 65,165113). thanks God! PSG people have not defeated the string theorist (their solution gives infinite number of unverse).

Types of Spin Liquid

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Physical Realizations

Experimental candidates for QSLs

- $ZnCu_3(OH)_6Cl_2$
  Herbertsmithite Kagome lattice
- Quasi-two dimensional Organic conductors of the BEDT-TTF like $\kappa-(ET)_2Cu_2(CN)_3$ (dmit salts)
- $Ba_3CuSb_2O_9$ triangular compunds
- $Na_4Ir_3O_8$ three-dimensional hyper Kagome lattice

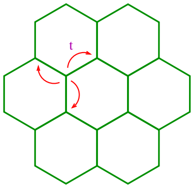
Figure: A sample of the mineral herbertsmithite. Credit: Rob Lavinsky/irocks.com

Section 2

Kitaev-Hubbard Model

Graphene non-int

Nearest neighbour hopping on the honeycomb lattice



$$\mathcal{H} = -t \sum_{<ij>_{\alpha},\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + h.c.$$

Additional spin dependent hopping

$$\mathcal{H} = - \sum_{<ij>_{\alpha},\sigma,\sigma'} c^{\dagger}_{i\sigma} P^{\alpha}_{\sigma,\sigma'} c_{j\sigma'} + h.c.$$

$$P^{\alpha}_{\sigma,\sigma'} = \frac{(t + t'\tau^{\alpha}_{\sigma\sigma'})}{2}$$

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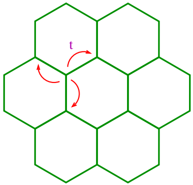

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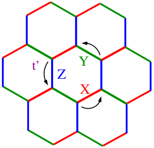

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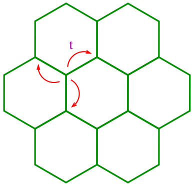

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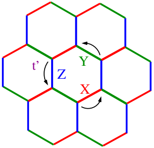

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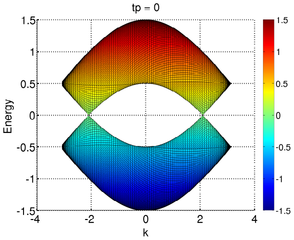
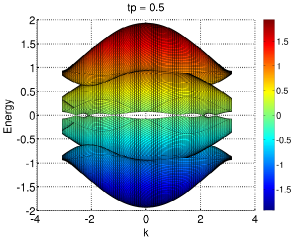
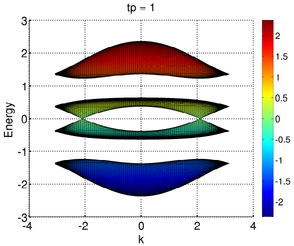
Spectra Kitaev Limit



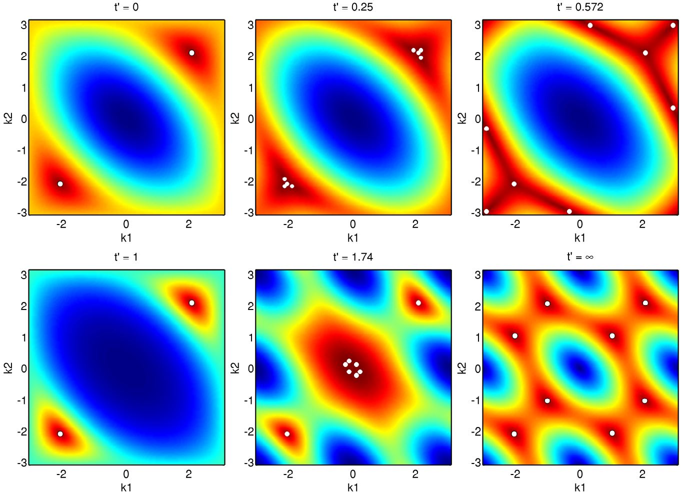


Overlap of the bands: $t' > 0.717$, a non-zero gap exists between the first and the second band for all k.

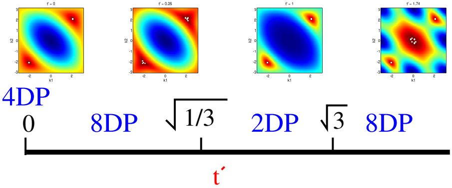


Energy Spectra

Dirac points are shown as the white dots in the second band

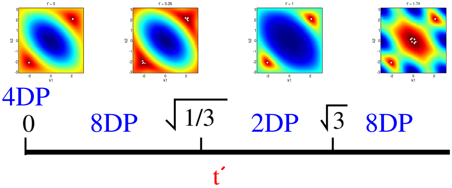


Phase Diagram



Topological Lifshitz transition: Topological as the fermi surface is changing as a function of t'. The density of states at the transition points shows a change in the behaviour.

Phase Diagram



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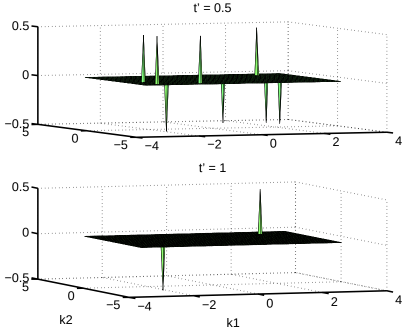
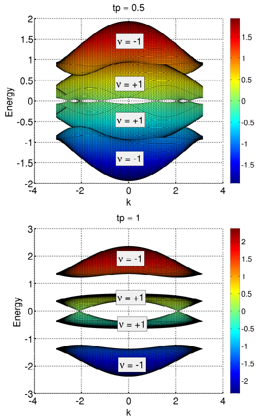
Pancharatnam-Berry Phase

Non-trivial topological properties





Chern number of the bands $-1, +1, +1, -1$.

Methods to be discussed

- Many quantum cluster methods are in order:

- Cluster Perturbation Theory (CPT)

- Variational Cluster Approximation (VCA) or (VCPT)

- Cluster Dynamical Mean Field Theory (CDMFT)

- VCA & CDMFT $\Rightarrow$ SEF approach (M. Potthoff)

- DCA $\Rightarrow$ momentum analog of CDMFT (will not be discussed)

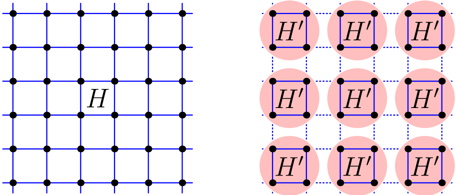
What is CPT ?

- Cluster extension of strong-coupling perturbation theory (SCPT) limited to lower order

  - The procedure is:

    - Choose a cluster tiling & write:

$$H = H' + V$$



A two D lattice & the corresponding four site clusters.

- Lattice Green function:

$$G^{-1}(\omega, \mathbf{k}) = G'^{-1}(\omega) - V(\mathbf{k})$$

CPT (cont.)

- Some transformations:

$$G^{-1}(\omega,\mathbf{k}) = G'^{-1}(\omega) - V(\mathbf{k})$$

Using:

$$G'^{-1}(\omega) = \omega - t' - \Sigma(\omega) \quad \& \quad G_0'^{-1}(\omega,\mathbf{k}) = \omega - t' - V(\mathbf{k})$$

The lattice Green function (GF) can be expressed in function of the

self-energy :

$$G^{-1}(\omega,\mathbf{k}) = G_0'^{-1}(\omega,\mathbf{k}) - \Sigma(\omega)$$

Supplemental ingredient to CPT

- Periodization prescription (PP) which applies to GF.

$$G_{per}(\mathbf{k},\omega) = \frac{1}{L}\sum_{\mathbf{RR'}} \exp[-i\mathbf{k}.(\mathbf{R}-\mathbf{R'})]G_{\mathbf{RR'}}(\tilde{\mathbf{k}},\omega)$$

  - PP conserves the diagonal piece of G & discards the rest.
  - This makes sense in as well as:

$$N(\omega) = \frac{-2}{N}\,\mathrm{Im}\,\sum_{\mathbf{k}} G_{(\mathbf{k},\omega)},$$

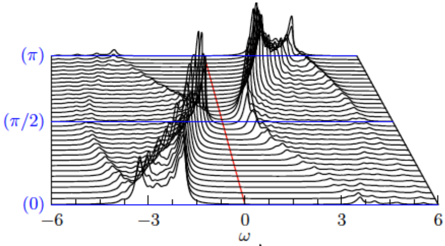
$A(\mathbf{k},\omega)$ partial trace of the diagonal part &

$$-2\,\mathrm{Im}\int \frac{d\omega}{2\pi}G(\omega) = 1$$

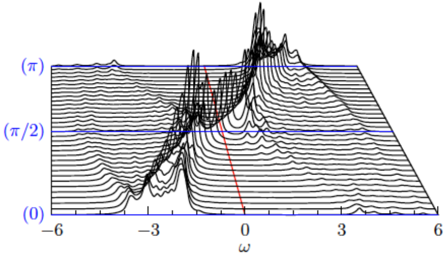
- Another PP applies Σ & follows the same procedure.

CPT results

- Green function periodization:



- Self-energy periodization:



CPT spectral function 1D, n=1, L=16, U=4, t=1

Sefl-energy functional approach

CPT: no successful to describe spontaneous broken symmetry.

But

$$H'_M = M \sum_{\mathbf{R}} \exp(i\mathbf{Q}.\mathbf{R})(n_{\mathbf{R}\ \sigma} - n_{\mathbf{R}\ -\sigma})$$

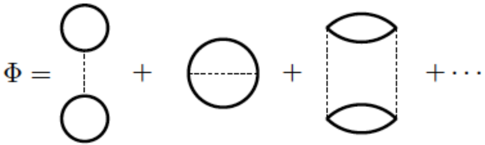
- How to set the value of the Weiss field M?
- This is the role of the SEF approach.

Self-energy functional approach (cont.)

- The approach starts with:

$$\Omega_t[G] = \Phi[G] - Tr[(G_{0t}^{-1} - G^{-1})G] + Tr\ln(-G)$$

where



- The Derivative is the self-energy

$$\frac{\delta \Phi[G]}{\delta G} = \Sigma$$

- $\Phi[G]$ is universal functional of G.

Properties of the Potthoff functional

$$\Omega_t[\Sigma] = F[\Sigma] - Tr\ln(-G_{0t}^{-1} + \Sigma) \qquad F[\Sigma] = \Phi[G] - Tr(\Sigma G)$$

- From Dyson equation: $$\frac{\delta\Omega_t[\Sigma]}{\delta\Sigma} = \frac{\delta\Omega_t[G]}{\delta G} = \Sigma - G_{0t}^{-1} + G^{-1} = 0$$

Type III approximation $\Leftrightarrow$ Universality of $F[\Sigma]$ & for cluster:

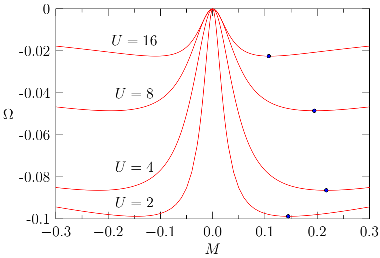
$$\Omega_{t'}[\Sigma] = F[\Sigma] - Tr\ln(-G'^{-1})$$

Finally the functional becomes:

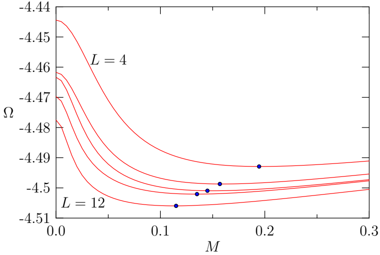
$$\Omega_t[\Sigma] = \Omega_{t'}[\Sigma] - T\sum_{\omega}\sum_{\mathbf{k}} \ln det[1 - V(\mathbf{k})G'(\omega)]$$

Setting Weiss filed value from Potthoff functional

- $\Omega(M)$ for various values of U,



- $\Omega(M)$ for various cluster sizes,



VCA (VCPT)

- Extension of CPT where some cluster parameters are set according PVP through the search for saddle points of $\Omega_t(\Sigma)$
- The Weiss fields allow for broken symmetries;
- Weiss fields do not coincide with the order parameter;
- Interactions are not factorized;
- Short-range correlations exactly treated.

Procedure in VCA

- Choose the Weiss field,
- Calculate the functional $\Omega_t(\Sigma)$
- Optimize the functional $\Omega_t(\Sigma)$ in the space of variational parameters,
- At the saddle point, calculate the properties of the model.

VCA Results: SC vs AF on the square lattice

$$O_{sc} = \sum_{rr'} \Delta_{rr'} c_{r\uparrow} c_{r'\downarrow} + Hc$$

s-wave:

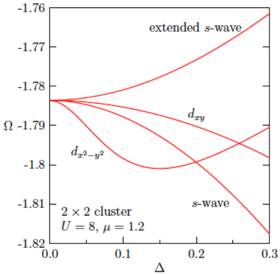
$$\Delta_{rr'} = \delta_{rr'}$$

$d_{x^2-y^2}$:

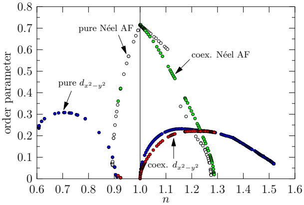
$$\Delta_{rr'} = \begin{cases} 1 & \text{if } r - r' = \pm \mathbf{e}_x \\ -1 & \text{if } r - r' = \pm \mathbf{e}_y \end{cases}$$

d_{xy}:

$$\Delta_{rr'} = \begin{cases} 1 & \text{if } r - r' = \pm(\mathbf{e}_x + \mathbf{e}_y) \\ -1 & \text{if } r - r' = \pm(\mathbf{e}_x - \mathbf{e}_y) \end{cases}$$



2x2 U=8, $\mu = 1.2$



M. Guillot MSc thesis

CDMFT

- CDMFT is a cluster extension of DMFT.
- Basic idea:
  - Model the effect of environment on the cluster,
  - Uses bath of uncorrelated orbitals,
  - Cluster's Hamiltonian:

$$H' = \sum_{\mu\nu} t_{\mu\nu} c^{\dagger}_{\mu} c_{\nu} + U \sum_{\mathbf{R}} n_{\mathbf{R}\uparrow} n_{\mathbf{R}\downarrow} + \sum_{\mu\alpha} \theta_{\mu\alpha} (c^{\dagger}_{\mu} a_{\alpha} + H.c) + \sum_{\alpha} \varepsilon_{\alpha} a^{\dagger}_{\alpha} a_{\alpha}$$

  - $\theta_{\mu\alpha}$ & ε_{α} to be set in self-consistency way.

CDMFT cont.

- Effect of bath in electron Green function:

$$\Gamma_{\mu\nu}(\omega) = \sum_{\alpha} \frac{\theta_{\mu\alpha}\theta^*_{\nu\alpha}}{\omega - \varepsilon_\alpha}$$

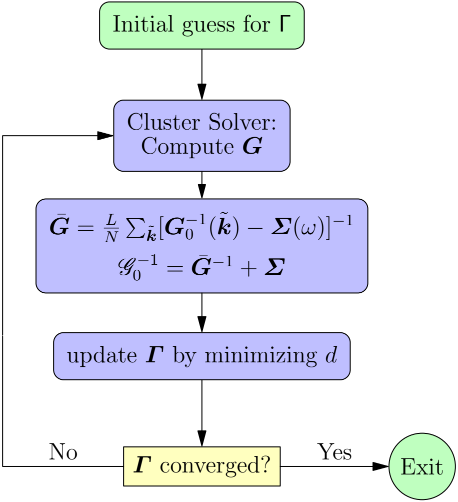
- Enters the cluster Green function as:

$$G'^{-1}(\omega) = \omega - t - \Gamma(\omega) - \Sigma(\omega)$$

CDMFT Procedure

- Guess value of $\theta_{\mu\alpha}$ & $\varepsilon_\alpha \Rightarrow \Gamma$
- Calculate $G'(\omega)$
- calculate $\bar{G}(\omega)$
- Minimize d:

$$d = \sum_{\omega\mu\nu} |(\omega + \mu - t' - \Gamma - g_0^{-1})_{\mu\nu}|^2$$

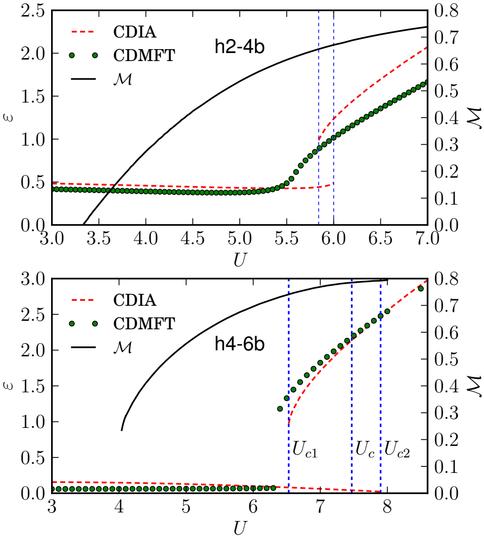


$$g_0^{-1}(\omega) = \bar{G}(\omega) + \Sigma(\omega)$$

CDIA (same procedure as VCA)

- Cluster extension of DIA
- What is exactly CDIA ?
  - Can take Weiss field (CDMFT cannot)
  - Can take bath (VCA cannot)
  - Close to CDMFT because the bath,
  - Close to VCA because sets values of $\theta_{\mu\alpha}$ & ε_{α} according to SEF approach: $\Rightarrow$ it must be more accurate the VCA & CDMFT

CDIA & CDMFT results



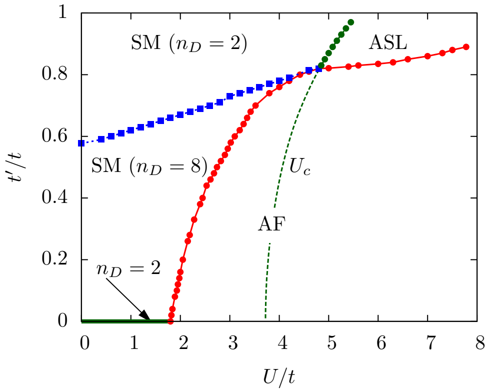
Hassan et all PRL (2013)

Section 4

Phase Diagram

Phase Diagram

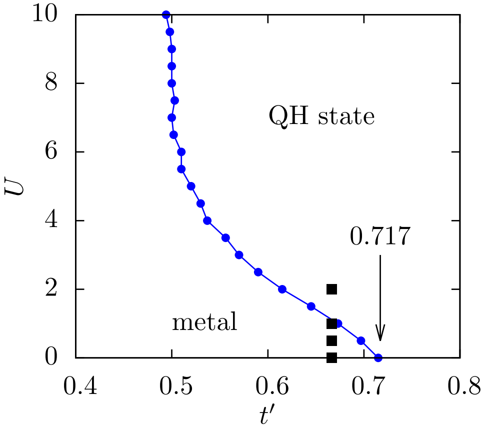
Phase Diagram at half-filling computed using CDIA and CDMFT



AF : Antiferromagnetic insulator
SM : Semi-Metal
ASL : Algebraic Spin Liquid

Phase Diag contd ...

At quarter filling we get the following Phase Diagram



Section 5

Effective Hamiltonian and Mean field theory

Effective Hamiltonian

The second order effective hamiltonian at $t = 1$ and $t' = 1$ is the Kitaev spin model.

$$\mathcal{H}_e^{(2)} = \frac{2}{U} \sum_{\langle ij \rangle_\alpha} S_i^\alpha S_j^\alpha$$

For non zero t' we get the Kitaev Heisenberg Hamiltonian.

$$\mathcal{H}_e^{(2)} = \sum_{\langle ij \rangle_\alpha} \left[\frac{(1 - t'^2)}{U} \vec{S}_i \cdot \vec{S}_j + \frac{2t'^2}{U} S_i^\alpha S_j^\alpha \right]$$

The fourth order effective hamiltonian

$$\mathcal{H}_e^{(4)} = \sum_{\substack{\langle ij \rangle_\alpha \\ \beta \neq \alpha}} \left[\frac{(t'^4 - 1)}{U^3} \mathbf{S}_i . \mathbf{S}_j - \frac{2t'^4}{U^3} S_i^\alpha S_j^\alpha - \frac{2t'^2}{U^3} (S_i^\alpha S_j^\beta + S_j^\alpha S_i^\beta) \right]$$

$$+ \sum_{\langle\langle ij \rangle\rangle_{\alpha\beta}} \left[\frac{(1 - t'^2)^2}{4U^3} \mathbf{S}_i . \mathbf{S}_j + \frac{t'^2 - t'^4}{2U^3} (S_i^\alpha S_j^\alpha + S_i^\beta S_j^\beta) + 3 \frac{t'^2}{U^3} S_i^\alpha S_j^\beta \right]$$

where $S_i = \sum_\alpha S_i^\alpha$.

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where $S_i = \sum_\alpha S_i^\alpha$.

Mean Field theory

We compute the gap in the spinon spectra we consider the hamiltonian

$$H = \mathcal{H}_e^{(2)} + \mathcal{H}_e^{(4)}$$

and we separate this hamiltonian into the Kitaev hamiltonian and the other spin terms.

$$H = \mathcal{H}_0 + \mathcal{H}_p; \qquad \mathcal{H}_0 = J \sum_{\langle ij \rangle_\alpha} S_i^\alpha S_j^\alpha$$

$\mathcal{H}_p$ contains all other spin terms other than the Kitaev term. We write the spin in terms of majorana fermions as

$$\sigma_i^\alpha = i c_i b_i^\alpha, \qquad \{c_i, c_j\} = 2\delta_{ij} \qquad \{b_i^\alpha, b_j^\beta\} = 2\delta_{\alpha\beta}\delta_{ij}, \qquad \{c_i, b_j^\alpha\} = 0$$

The physical subspace is defined by the constraint

$$c_i b_i^x b_i^y b_i^z |\psi\rangle_{\text{phys}} = |\psi\rangle_{\text{phys}}$$

Mean Field theory

We compute the gap in the spinon spectra we consider the hamiltonian

$$H = \mathcal{H}_e^{(2)} + \mathcal{H}_e^{(4)}$$

and we separate this hamiltonian into the Kitaev hamiltonian and the other spin terms.

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Mean Field contd...

In terms of these Majorana fermions, the leading order Hamiltonian is,

$$\mathcal{H}_0 = J \sum_{\langle ij \rangle_\alpha} i c_i c_j i b_i^\alpha b_j^\alpha$$

The decoupling of the spinon and gauge field sectors is represented by

$$\sigma_i^\alpha \sigma_j^\beta = -i c_i c_j \; i b_i^\alpha b_j^\beta \approx -i c_i c_j B_{ij}^{\alpha\beta} - i C_{ij} b_i^\alpha b_j^\beta + C_{ij} B_{ij}^{\alpha\beta}$$

with the self-consistency equations

$$B_{ij}^{\alpha\beta} \equiv \langle i b_i^\alpha b_j^\beta \rangle \qquad C_{ij} \equiv \langle i c_i c_j \rangle$$

Mean Field contd...

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$$B_{ij}^{\alpha\beta} \equiv \langle i b_i^\alpha b_j^\beta \rangle \qquad\qquad C_{ij} \equiv \langle i c_i c_j \rangle$$

Mean Field contd...

The mean field Hamiltonian at $t' = 1$ is,

$$H_{MF} = H^b_{MF} + H^c_{MF}$$

with the spinon hamiltonian as

$$H^c_{MF} = \frac{1}{4} \sum_{\mathbf{k} \in HBZ} \begin{pmatrix} c^\dagger_{\mathbf{k}_A} & c^\dagger_{\mathbf{k}_B} \end{pmatrix} \begin{pmatrix} iv_1(\mathbf{k}) & iu(\mathbf{k}) \\ -iu^*(\mathbf{k}) & iv_2(\mathbf{k}) \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}_A} \\ c_{\mathbf{k}_B} \end{pmatrix}$$

$$u(\mathbf{k}) = \sum_\alpha e^{-i\vec{k}\cdot\vec{e}_\alpha} \left(J\eta + \gamma_1 \sum_{\beta \neq \alpha} B^{\alpha\beta}_\alpha \right)$$

$$v_1(\mathbf{k}) = 2ib_1\gamma_2 \sum_\alpha \sin(\vec{k}\cdot\vec{e}_\alpha) \qquad v_2(\mathbf{k}) = -2ib_2\gamma_2 \sum_\alpha \sin(\vec{k}\cdot\vec{e}_\alpha)$$

We solve the mean field equations self consistently to obtain the spinon spectra to be gapless from $U = 2 - \infty$.

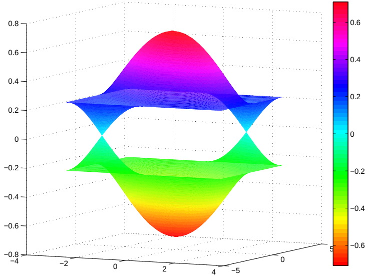

Figure: Spinon dispersion relation at $U = 2$.

This behaviour is seen at different t' as well.

Section 6

Summary and Conclusion

Summary

- The Kitaev-Hubbard model is a model on the honeycomb lattice with Spin-dependent hopping which breaks time-reversal symmetry.
- Multiple Dirac points transtions occur at which the density of states shows a sharp behavioural change.
- The bands have non-zero Chern number. But the sum of the Chern numbers at half-filling is zero.
- Bloch-Zener oscillations probe the Dirac points in the model.
- Rotating cloud shows the effect of the non-zero PB curvature of the bands
- Phase diagram at half filling revealed a Stable Algebraic Spin Liquid phase using CDIA and CDMFT.
- Phase diagram at quarter filling revealed a QH state.

Still more can be explored ...

References

Students



Collaborators


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