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Topological condensed matter physics
Problem set 4

Summer term 2016

1. Phase diagram of the BHZ model **1 Point**

Let us consider the Bloch matrix of the Bernevig–Hughes–Zhang model which is used to described the topological insulator state in the HgTe quantum wells. Defined for a square lattice with two orbitals per site (the orbital space is denoted by σ^α), the Bloch matrix reads

$$H_{\mathrm{BHZ}}(k_x, k_y) = \begin{pmatrix} h(\boldsymbol{k}) & 0 \\ 0 & h^\star(-\boldsymbol{k}) \end{pmatrix} \tag{1}$$

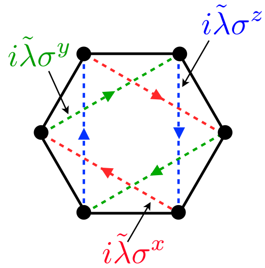
where $h(\boldsymbol{k}) = \boldsymbol{d}(\boldsymbol{k})\cdot\boldsymbol{\sigma}$ with $d_1(\boldsymbol{k}) = \sin(k_x)$, $d_2(\boldsymbol{k}) = \sin(k_y)$, and $d_3(\boldsymbol{k}) = 2B + M - B[\cos(k_x) + \cos(k_y)]$.

a) **1 Point**

Determine the phase diagram of the BHZ model depending on the parameter M/B.

2. Sodium Iridate model for $\mathbb{Z}_2$ topological insulators **4 Points**

The sodium iridate (SI) model defined on the honeycomb lattice is a variant of the Kane-Mele model. In contrast to the Kane-Mele model, the second-neighbor spin-orbit hoppings are different on second-neighbor bond directions, see the following figure:



After Fourier transformation, the Hamiltonian of the SI model reads

$$H_{\mathrm{SI}} = \sum_{\boldsymbol{k}} \Psi^\dagger(\boldsymbol{k}) \left[\sum_l g_l(\boldsymbol{k})\Gamma_l + \sum_{lm} g_{lm}(\boldsymbol{k})\Gamma_{lm} \right] \Psi(\boldsymbol{k}) \tag{2}$$

with the four-component spinor $\Psi^\dagger(\boldsymbol{k}) = \left(a^\dagger_{\boldsymbol{k}\uparrow}, b^\dagger_{\boldsymbol{k}\uparrow}, a^\dagger_{\boldsymbol{k}\downarrow}, b^\dagger_{\boldsymbol{k}\downarrow}\right)$, appropriately chosen functions $g_l(\boldsymbol{k})$ and $g_{lm}(\boldsymbol{k})$, and the five 4×4 matrices Γ_l $(l = 1, \ldots, 5)$ are the generators of a Clifford algebra. They fulfill

$$\{\Gamma_l, \Gamma_m\} = 2\delta_{lm} \quad \text{and} \quad \Gamma_{lm} = \frac{1}{2i}[\Gamma_l, \Gamma_m] \ . \tag{3}$$

In this general form, graphene is recovered for $g_1(\boldsymbol{k}) = t(1+2\cos(x)\cos(y))$ and $g_{12}(\boldsymbol{k}) = -2t\cos(x)\sin(y)$ with $x = k_x a/2$ and $y = \sqrt{3}k_y a/2$ (all other g's are zero).
For additional $g_{15}(\boldsymbol{k}) = \lambda_{\mathrm{KM}}(2\sin(2x) - 4\sin(x)\cos(y))$, one obtains the minimal version of the Kane-Mele model. Now the SI model requires the three additional functions $g_{13}(\boldsymbol{k}) = 2\lambda_{\mathrm{SI}}\sin(x+y)$, $g_{14}(\boldsymbol{k}) = 2\lambda_{\mathrm{SI}}\sin(x-y)$, and $g_{15}(\boldsymbol{k}) = 2\lambda_{\mathrm{SI}}\sin(2x)$. Eventually we add the staggered sublattice potential $g_2 = M$.

a) **2 Points**

Consider the SI model (*i.e.*, $\lambda_{\text{KM}} \equiv 0$). Determine the relation between M and λ_{SI} for which the bulk gap closes and the ground state can change from topologically trivial to non-trivial and/or vice versa. *Hint:* Which are the only points in the Brillouin zone where the gap can close?

b) **2 Points**

In the lecture we proved that the Kane-Mele model is a $\mathbb{Z}_2$ topological insulator. Show that also the SI model is in the same topological class: Show that the bulk gap does not close while adiabatically transforming the TI phase of the Kane-Mele model to the one of the SI model. That is, consider the gap-closing condition for variabel α,

$$\alpha\lambda_{\text{SI}} + (1-\alpha)\lambda_{\text{KM}} \ , \qquad \alpha \in [0,1] \ . \tag{4}$$

3. Strong coupling limit and the Heisenberg model **2 Points**

Consider a real nearest-neighbor hopping on an arbitrary lattice,

$$H_0 = -t \sum_{ij} \sum_{\sigma=\uparrow,\downarrow} c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.} \ . \tag{5}$$

If we want to describe the effect of Coulomb repulsion between the electrons, this can be accomplished in the simplest way using a Hubbard interaction,

$$H_I = U \sum_i n_{i\uparrow} n_{i\downarrow} \ , \tag{6}$$

where $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ is the number operator. At half filling, *i.e.*, one particle per lattice site, and for strong U hopping processes of the electrons are suppressed. This is the strong coupling limit where only the spin degree of freedom of the electrons remains.

a) **1 Point**

Show that (5) corresponds for very large U (formally, one performs second order perturbation theory in $1/U$) to the spin Hamiltonian

$$H_{\text{spin}} = J \sum_{ij} \left[\frac{1}{2} \left(S^+_i S^-_j + S^-_i S^+_j \right) + S^z_i S^z_j \right] \tag{7}$$

with $J = (4t^2)/U$. This is the isotropic Heisenberg model. Note that the spin operators can be expressed through fermionic operators as $S^+_i = c^\dagger_{i\uparrow} c_{i\downarrow}$ and $S^z_i = (n_{i\uparrow} - n_{i\downarrow})/2$.

b) **1 Point**

How does the resulting spin Hamiltonian change when imaginary, spin-dependent hopping is considered instead of (5)? As an concrete example, consider the Kane-Mele term

$$H'_0 = i\lambda_{\text{KM}} \sum_{\langle\langle ij \rangle\rangle} \nu_{ij} c^\dagger_{i\alpha} \sigma^z_{\alpha\beta} c_{j\beta} \tag{8}$$

as introduced in the lecture.

In case of questions or lack of clarity please write us an email for clarification or further advice.