ICFP M2 2022/2023

Condensed Matter Theory

Homework Assignment

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Please note:

This homework is due in the first exercise group (TD) after the ICFP research seminars, i.e. on **24 November 2022**. Please hand in your solutions of parts A, B and C of this homework on **separate sheets of paper** in order to facilitate grading: Mark the sheets by the letter corresponding to that part (A, B, or C) in a well-visible manner, and do not forget to write your name on all sheets.

A. The Rice-Mele model

The Rice-Mele (RM) model is defined on the same chains as the Su-Schrieffer-Heeger (SSH) model. As a reminder from exercise sheet 4, the SSH model is defined on a finite one-dimensional chain of N unit cells, with each cell consisting of two sites, A and B. The SSH Hamiltonian reads as

$$\mathcal{H}_N = t\sum_{j=1}^{N}(|j,A\rangle\langle j,B| + \text{h.}c.) + t'\sum_{j=1}^{N-1}(|j+1,A\rangle\langle j,B| + \text{h.}c.).$$

The RM model is obtained by adding the term

$$\mathcal{H}_{N,m} = m\sum_{j=1}^{N}\left(|j,A\rangle\langle j,A| - |j,B\rangle\langle j,B|\right)$$

to the SSH model assuming $m \neq 0$.

(a) Find the RM matrix $\hat{\mathcal{H}}_N^{\text{RM}}(k) = \hat{\mathcal{H}}_N(k) + \hat{\mathcal{H}}_{N,m}(k)$. Find the bandstructure of $\hat{\mathcal{H}}_N^{\text{RM}}(k)$ and the bandgap. Assuming $m \neq 0$, is there still a transition in the model?

(b) Does this Hamiltonian anticommute with any k-independent matrix ? What are the implications for topological properties as we discussed for the SSH model?

(c) To study a single eigenstate with both $t,t' > 0$, we consider a half-infinite SSH chain defined by $\mathcal{H}_\infty = \lim_{N\to\infty}\mathcal{H}_N$. Assume that there is an eigenstate $|\psi_0\rangle$ at zero energy, and find it explicitly. [Hint: Write $|\psi_0\rangle$ as a linear combination of the states $|n,\alpha\rangle$ with $\alpha = A,B$ and $n = 1,\cdots,\infty$ and solve the Schroedinger equation as a system of linear equations in the coefficients]. For which regime of t,t' is this a valid state? What is the value of exponential decay length $\xi(t,t')$ of $|\psi_0\rangle$? Discuss the behavior of $\xi(t,t')$ near $t = t'$.

(d) Find the exact change in energy of the edge state (when $t' > t$) in the RM model $\mathcal{H}_\infty^{\text{RM}} \equiv \mathcal{H}_\infty + \lim_{N\to\infty}\mathcal{H}_{N,m}$, considering $\mathcal{H}_{N,m}$ as a perturbation. Is it still a zero mode?

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B. Spinful graphene

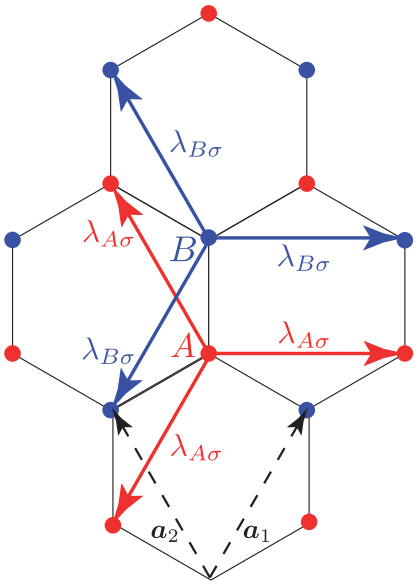

Figure 1: Graphene lattice in real space, with arrow depicting all the spin-dependent next-nearest-neighbor hoppings assigned to one unit-cell (the marked A,B). An arrow pointing from site i to site j, labeled by $\lambda_{\alpha\sigma}$ represents the term $\lambda_{\alpha\sigma}c^\dagger_{\alpha,j,\sigma}c_{\alpha,i,\sigma}$, where $\alpha \in \{A,B\}$ is the type of sites i,j.

In this problem we consider a more realistic model of graphene by addressing the spin-1/2 nature of electrons and by adding next-nearest neighbor hoppings. Together these features allow us to better study transitions in Dirac systems, and the role of spin-orbit coupling in graphene. We will use the tight-binding lattice model Hamiltonian $H = H_t + H_m + H_\lambda$, with:

$$H_t = \sum_{\sigma=\uparrow,\downarrow}\sum_{R,\delta} t_\sigma c^\dagger_{B,R+\delta,\sigma}c_{A,R,\sigma} + h.c. \tag{1}$$

$$H_m = \sum_{\sigma=\uparrow,\downarrow}\sum_{R} m_\sigma (c^\dagger_{A,R,\sigma}c_{A,R,\sigma} - c^\dagger_{B,R,\sigma}c_{B,R,\sigma}) \tag{2}$$

$$H_\lambda = \sum_{\sigma=\uparrow,\downarrow}\sum_{\langle\langle R,R'\rangle\rangle} \lambda_{\alpha\sigma}c^\dagger_{\alpha,R',\sigma}c_{\alpha,R,\sigma} + h.c., \tag{3}$$

where the operator $c^\dagger_{\alpha,R,\sigma}$ creates an electron on site $\alpha = A,B$ in unit-cell $\vec{R}$, and with spin $\sigma = \uparrow , \downarrow$. We further focus on spin-independent nearest-neighbor hopping $t_\sigma \equiv t > 0$ and on-site potential terms ($m_\sigma \equiv m$, so that $H_t + H_m$ becomes two independent copies of the spinless graphene you studied in TD and main lecture. More precisely: $R \equiv \vec{R} \equiv \vec{R}_A$ is the position of the unit-cell defined to coincide with the position of A atom in that unit-cell (hence use the inverse Fourier transform $c^\dagger_{\alpha,k,\sigma} = \int_{BZ}\frac{\mathrm{d}^2k}{2\pi}\exp(-i\vec{k}\cdot\vec{R})c^\dagger_{\alpha,k,\sigma}$); the sum over $\vec{\delta}$ ensures that hoppings to all three nearest neighbors of A are included. However, the H_λ adds four new complex spin-dependent next-nearest neighbor hoppings $\lambda_{\alpha\sigma} \in \mathbb{C}$, $\alpha = A,B$, $\sigma = \uparrow , \downarrow$, and the precise definition of the next-nearest neighbor terms $\langle\langle R,R'\rangle\rangle$ is in Fig. 1.

(a) What is the Hamiltonian in momentum space? What is the 2x2 matrix spin-dependent Hamiltonian h_k^σ for momentum k?

(b) The antiunitary time-reversal operator $\mathcal{T}$ for spin$-\frac{1}{2}$ electrons acts in the following way:

$$\mathcal{T} z c_{\alpha,R,\uparrow} \mathcal{T}^\dagger = +z^* c_{\alpha,R,\downarrow}, \tag{4}$$

$$\mathcal{T} z c_{\alpha,R,\downarrow} \mathcal{T}^\dagger = -z^* c_{\alpha,R,\uparrow}, \tag{5}$$

for a complex number z. What are the constraints on t,m,$\lambda_{\alpha\sigma}$ when time-reversal symmetry is imposed on the Hamiltonian?

(c) What is the 2x2 matrix $\mathcal{H}_q^{\sigma,\xi}$ for the time-reversal symmetric Hamiltonian at small momenta $|\vec{q}| \ll |\vec{K}_D|$ near the Dirac points $\xi\vec{K}_D$, $\xi = \pm 1$?

(d) What is the energy dispersion of $\mathcal{H}_q^{\sigma,\xi}$?

(e) The unitary spatial inversion operator $\mathcal{I}$ for spin$-\frac{1}{2}$ electrons acts in the following way:

$$\mathcal{I} z c_{A/B,k,\sigma} \mathcal{I}^\dagger = +z c_{B/A,R-k,\sigma}, \tag{6}$$

for a complex number z. What are the constraints on t,m,$\lambda_{\alpha\sigma}$ for the spin-dependent Hamiltonian h_k^σ to be inversion-symmetric as well as time-reversal symmetric? Can a gap open at the Dirac points under these conditions? What can you say about the symmetry protection of the Dirac cones in presence of spin?

(f) As the Hamiltonian parameters m,$\lambda_{\alpha\sigma}$ vary, a topological band transition (TBT) leading to a change of topological properties of the bands, can only occur when bands touch at a certain momentum k_0. A transition requires a mixing among band states as parameters change, hence we can disregard crossings of bands with different conserved quantum numbers and crossings due to rigid shifts of bands, i.e., due to Hamiltonian terms $\propto \mathbb{1}$. At which parameter values and at which momenta are TBT possible in the time-reversal and inversion symmetric low-energy Hamiltonian $\mathcal{H}_q^{\sigma,\xi}$? How many topologically different phases of gapped graphene do you think there are?

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C. Green's functions

(a) Consider electrons of a one-dimensional chain of Hydrogen atoms (with periodic boundary conditions) within a tight-binding approximation retaining nearest-neighbor hopping t, as in the lecture. In second quantized notation denote the creation/annihilation operators by $(c^\dagger_{i,\sigma}, c_{i,\sigma})$, where i is the site index of the chain and σ is the spin of the electron. Consider the retarded Green's function

$$G^R(\mathbf{k},\sigma,t) \equiv -i\theta(t)\langle\{c_{\mathbf{k},\sigma}(t)\,,\, c^\dagger_{\mathbf{k},\sigma}(0)\}\rangle,$$

where $\mathbf{k}$ is the wave-vector of the electrons, $\langle\hat{\mathcal{O}}\rangle \equiv (1/Z)\sum_n e^{-\beta E_n}\langle n|\mathcal{O}|n\rangle$, and $|n\rangle$ are the energy eigenstates of the Hamiltonian. Neglecting any Coulomb interactions, calculate the Fourier transform of the above quantity,

$$G^R(\mathbf{k},\sigma,\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} G^R(\mathbf{k},\sigma,t),$$

for this system by at least two different methods of your choice. (You may e.g. use the Lehmann representation, or you may calculate G^R in time and then Fourier transform etc...). Calculate the spectral function and make a sketch of what you would expect to measure during a photoemission or inverse photoemission experiment.
A small caveat : The retarded Green's function slightly differs from the time-ordered Green's function defined during the lecture. How does the Lehmann representation for the retarded one look like?

(b) Consider now a single-site problem (i.e., not a chain) with an isolated Hydrogen atom whose electrons are described by the Hamiltonian $H = \epsilon(n_\uparrow + n_\downarrow) + U(n_\uparrow - \frac{1}{2})(n_\downarrow - \frac{1}{2})$. Give an interpretation of the two terms. Convince yourself that for $\epsilon = 0$ the system is half-filled. Calculate the retarded Green's function of this system which is given by

$$G^R(\sigma,t) \equiv -i\theta(t)\langle\{c_\sigma(t)\,,\, c^\dagger_\sigma(0)\}\rangle,$$

and its Fourier transform $G^R(\sigma,\omega)$. Note, since this is a single-site problem there is no site index, or wave-vector index. Calculate also the corresponding non-interacting ($U = 0$) Green's function $G^R_0(\sigma,\omega)$ and deduce the self-energy (defined by $\Sigma(\sigma,\omega) = G^R_0(\sigma,\omega)^{-1} - G^R(\sigma,\omega)^{-1}$). Calculate the spectral function and make a sketch of what you would expect to measure during a photoemission or inverse photoemission experiment.

(c) Assume now that the self-energy calculated in the previous task (b) can be used as an approximation to the self-energy of an interacting 1d chain problem. Write down the retarded Green's function $G^R(\mathbf{k},\sigma,\omega)$ of the 1d chain resulting from making this approximation. Can you determine its poles? Calculate and sketch the spectral function. Comment on the approximation made. Under which circumstances would you expect it to describe your system qualitatively correctly?

(d) Now make a different approximation to the self-energy of the retarded Green's function. Assume it to have the form $\Sigma^R(k,\omega) = C + Z_{\mathbf{k}}^{-1}\omega - i\Gamma\omega^2$. What are the dimensions of the parameters $(C, Z_{\mathbf{k}}, \Gamma)$? Determine whether Γ is a positive or negative quantity. Assuming the system is in the "normal Fermi liquid regime", what can you say about the coefficients C and Z_k^{-1} Calculate the retarded Green's function $G^R(\mathbf{k},\sigma,\omega)$ of the 1d chain using this self-energy. Deduce the spectral function.

In reality, the 1d chain system is not in the Fermi liquid regime. Nevertheless, the above form allows us to understand the modifications brought about by Fermi liquid-like self-energies onto band-like systems.
The approximation of using an atomic-like self-energy as in part c above is known under the name "Hubbard-1" approximation[1].

[1] J. Hubbard, *Proc. Roy. Soc. London A* **276** 238 (1963)