Homework #3 — PHYS 625 — Spring 2021
Deadline: Monday, March 22, 2020, by email to masoudma@umd.edu before class

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Do not forget to write your name and the homework number!

Tight-binding models. Single-particle Green's function

1. Band structure for a particle hopping on a square lattice

Consider an infinite square lattice with lattice spacing a and with discrete translation symmetry $\vec{a} \equiv (a_x, a_y) = (a, a)$. Consider fermionic particles (e.g., electrons) hopping on the lattice, described by the following (nearest-neighbor) Hamiltonian,

$$\hat{H}_{sq} = -t \sum_{\langle nm \rangle} \hat{c}_n^\dagger \hat{c}_m + \text{H.c.} \tag{1}$$

where, $\langle nm \rangle$ denote nearest-neighbor lattice sites.

(a) Calculate the band structure of the model $E(k)$.

(b) Provide an example of a perturbation to or modification of the Hamiltonian that would give rise to a gap in the spectrum. Note that there is no unique solution to this problem, there are in fact infinite number of perturbations that would result in a gap.

2. Band structure of a spinless graphene

Graphene has a two dimensional honeycomb lattice structure composed of regular hexagons as shown in Fig.1. Consider the nearest-neighbor hopping Hamiltonian for spinless graphene,

$$\hat{H}_{sq} = -t \sum_{\langle nm \rangle} \hat{a}_n^\dagger \hat{b}_m + \text{H.c.} \tag{2}$$

where, $\langle nm \rangle$ denote nearest-neighbor lattice sites on the honeycomb lattice and a, b are the electron annihilation operators on the A and B sublattice, respectively.

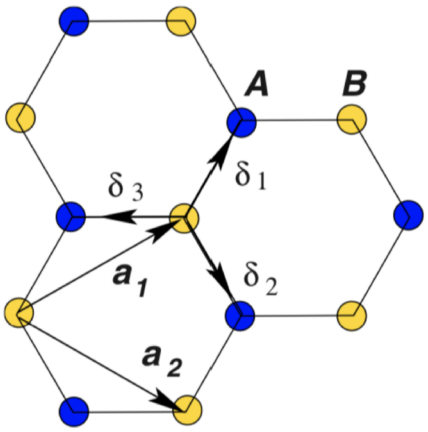

Figure 1: The sub-lattices in graphene are color-coded differently. $\vec{a}_1$ and $\vec{a}_2$ are the lattice unit vectors, and δ_i, $i = 1, 2, 3$ are the nearest-neighbor vectors. Let $||\delta_{1,2,3}|| = a \implies \vec{a}_1 = \frac{a}{2}(3, \sqrt{3}), \vec{a}_2 = \frac{a}{2}(3, -\sqrt{3})$

(a) Prove the existence of Dirac points in the spectrum, defined as a point in the Brillouin zone, where the density of state vanishes, while electron group velocity $v = \frac{d\epsilon(k)}{dk}$ remains finite. How many nonequivalent Dirac points are in the model?

(b) Calculate the band structure of the model $E(\vec{k})$. You can use numerical simulations (e.g. mathematica or Matlab or any other computer program) to plot the band structure. If you are unable to derive/plot the full band structure, just derive the asymptotic form of the band structure near the Dirac points.

3. In the lectures, we derived the following equation for the scattering amplitude operator

$$\hat{F} = \hat{V} + \hat{V}\hat{G}_0\hat{F}, \tag{3}$$

which is valid in any representation for any scattering potential. *E.g.*, in position representation it should be understood as an equation for the Kernel, $F(\mathbf{r}, t; \mathbf{r}', t')$ (the same holds for all operators involved). The action of an operator and the operator products are defined in a natural way (as a "continuum version" of a matrix product).

Derive the explicit form that Eq. (3) takes in energy-momentum representation.

4. Using the toy diagram tecninque developed in the lectures, derive the first correction to the Born approximation formula for the scattering amplitude. Draw the relevant diagram and write down the correpsonding equation in momentum representation.

5. In 1956, Leon Cooper considered the problem of electrons experiencing an attractive force, when their momenta lie within a thin shell near the Fermi surface. He showed that this interaction leads to the formation of bound states (now known as Cooper pairs) for an arbitrarily weak attractive force. His paper (`https://journals.aps.org/pr/abstract/10.1103/PhysRev.104.1189`) was the basis of the follow-up work

of Bardeen, Cooper, and Schrieffer, who were later awarded Nobel prize for the development of the theory superconductivity `http://nobelprize.org/nobel_prizes/physics/laureates/1972/`.

Consider the two-particle problem in which the particles experience a constant attractive potential, $-V_0$, if their momenta lie within a thin shell defined by

$$k_0 - \delta k < \{|\mathbf{k}_1|, |\mathbf{k}_2|\} < k_0 + \delta k$$

with $\delta k \ll k_0$ and do not interact otherwise.

Derive the Schrödinger equation in momentum space corresponding to this problem, solve it for the bound state (Cooper pair), and determine its binding energy. You may follow the famous work of Cooper, but are asked explain all calculations.

6. Bonus problem (not required): Bernevig-Hughes-Zhang (BHZ) model

Consider the BHZ model, introduced in class, with the 4×4 Bloch Hamiltonian defined as follows

$$\hat{H}_{BHZ} = \begin{pmatrix} \hat{h}_{\boldsymbol{p}} & 0 \\ 0 & \hat{h}^*_{-\boldsymbol{p}} \end{pmatrix} \tag{4}$$

where, $\hat{h}_{\boldsymbol{p}} = \epsilon_{\boldsymbol{p}}\hat{\mathbb{1}} + \vec{d}_{\boldsymbol{p}} \cdot \hat{\vec{\tau}}$, where the spin-orbit-coupling vector is $\vec{d}_{\boldsymbol{p}} = (Ap_x, Ap_y, M_p)$ and $\epsilon_{\boldsymbol{p}}$ is the spin-independent part of the electron dispersion. $M_p = M - Bp^2$ is the momentum-dependent Dirac mass, $\hat{\vec{\tau}} = (\hat{\tau}_x, \hat{\tau}_y, \hat{\tau}_z)$ is the vector of Pauli matrices and $\hat{\mathbb{1}}$ is a 2×2 unit matrix and A,B, and M are constant parameters.

(a) Plot the band structure of the BHZ model.

(b) Find the eigenstates, $|u_n(\boldsymbol{p})\rangle$ of one of the blocks of the BHZ Hamiltonian (where n is the band index; e.g., we can define $n = -1$ for the lower - valence - band and $n = +1$ for the upper - conduction - band).

(c) Calculate the Berry connection for the valence band (occupied in the insulating state) of one of the blocks,

$$\boldsymbol{A}(\boldsymbol{p}) = \langle u(\boldsymbol{p}) | \partial_{\boldsymbol{p}} u(\boldsymbol{p}) \rangle \tag{5}$$

Here, the band index is omitted for brevity.

(d) Calculate the corresponding Berry curvature in the valence band.

$$B(\boldsymbol{p}) = \mathrm{curl}\boldsymbol{A}(\boldsymbol{p}) \tag{6}$$

(e) Calculate the Chern number of the valence band of one of the blocks, by integrating the Berry curvature, for $M = B = +1$ and $B = -M = 1$.