Homework #2 — PHYS 625 — Spring 2018
Deadline: Wednesday, February-21, 2017, in class

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

Berry phase and band structures

1. **Berry phase of a spin-1/2 particle in a magnetic field.**
Consider the Hamiltonian of a spin-1/2 particle coupled to a time-dependent (slowly varying) Zeeman magnetic field $\vec{B}(t)$ (see lectures; below, we set the particle's magnetic moment to one),

$$\hat{\mathcal{H}}(t) = \vec{\mathbf{B}}(t) \cdot \hat{\vec{\boldsymbol{\sigma}}} \tag{1}$$

where, $\vec{\mathbf{B}}(t) = B\vec{\mathbf{n}}(t)$ (with B being a time-independent constant and $\vec{\mathbf{n}}(t)$ time-dependent *unit* vector) and $\hat{\vec{\boldsymbol{\sigma}}}$ is a vector of Pauli matrices. Assume that the system is initialized in the ground state at $t = 0$.

   (a) Write down an operator that rotates spin-1/2 by an angle χ around the vector $\vec{\mathbf{n}}$ and use this operator to derive the eigenstates of the Hamiltonian given above.

   (b) Calculate the Berry connection $\vec{\mathbf{A}}(\theta, \phi)$ in spherical coordinates. Assume spherical coordinates θ, ϕ to be defined by,

$$\vec{\mathbf{B}}(t) \equiv (B_x, B_y, B_z) = B(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta).$$

   Work out the technical details of the calculation that was outlined in the lectures.

   (c) Calculate the Berry curvature $F_{\theta\phi}$ and show that the degeneracy point $B = 0$ serves as a monopole of the Berry flux. Work out the technical details of the calculation that was outlined in the lectures.

   (d) Calculate the Berry phase γ for a closed path (i.e. $\vec{\mathbf{B}}(0) = \vec{\mathbf{B}}(T)$) traced out by $\vec{\mathbf{B}}(t)$ on the surface of the sphere with radius B, and show that $\gamma = \Omega/2$ where, Ω is the solid angle enclosed by this path. Work out the technical details of the calculation that was outlined in the lectures.

2. **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 a fermionic particles (e.g., electrons) hopping on the lattice, described by the following (nearest-neighbor) Hamiltonian

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

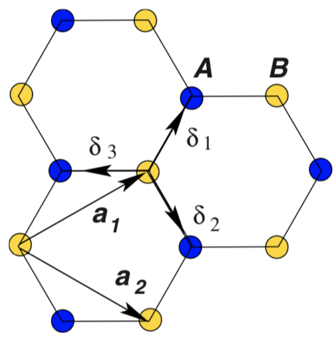

Figure 1: The sub-lattices in graphene are color-coded differently. $\mathbf{a_1}$ and $\mathbf{a_2}$ are the lattice unit vectors, and $\delta_i, i = 1, 2, 3$ are the nearest-neighbor vectors. Let $||\delta_{1,2,3}|| = a \implies \mathbf{a_1} = \frac{a}{2}(3, \sqrt{3}), \mathbf{a_2} = \frac{a}{2}(3, \sqrt{3})$

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

(a) Calculate the band structure of the model $E(\mathbf{k})$

(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.

3. 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,

$$\hat{H}_{hc} = -t \sum_{\langle nm \rangle} \hat{a}_n^\dagger \hat{b}_m + \text{H.c.} \tag{3}$$

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.

(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 $E(\mathbf{k})$. 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.