8.513 Problem Set # 3

Problems:

1. (10 pts) **The dynamics of a particle with spin-orbit coupling**
   The spin-1/2 particle is described by the following Hamiltonian

$$\hat{H} = \frac{1}{2m}\hat{\boldsymbol{p}}^2 + g\sigma^i \hat{p}_i + V(\hat{\boldsymbol{x}})$$

   where $i = x, y, z$ are the three directions of space and $g > 0$. The Pauli matrices σ^i act on the spin index of the particle. $V(\boldsymbol{x})$ is the external potential. (Remark: The spin-orbital coupling as given by this Hamiltonian implies the absence of inversion symmetry $\boldsymbol{x} \to -\boldsymbol{x}$. While unphysical for free space, this form of spin-orbit Hamiltonian can be realized in certain semiconductor crystals, in both two and three dimensions.)

   (a) Assume $V(\boldsymbol{x}) = 0$. Find the energy $\epsilon_{\boldsymbol{p}}$ of the lowest energy state with momentum $\boldsymbol{p}$. We denote such a state as $|\boldsymbol{p}\rangle$, and its wave function as $\psi_{\boldsymbol{p}}$.

   (b) A beam of particles is in a region with $V(\boldsymbol{x}) = 0$ where the particles are in the $|\boldsymbol{p}\rangle$ state defined above with $\boldsymbol{p}$ in the z direction: $\boldsymbol{p} = p\boldsymbol{z}$ and $p > gm$ (here $\boldsymbol{z}$ is the unit vector in the z direction). The beam strikes a hard wall which occupies the region with $z > 0$. The hard wall can be modeled by an infinite potential $V(\boldsymbol{x}) = +\infty$. What is the energy, the momentum, and the velocity of the reflected particles. (Hint: the reflection on the hard wall conserves the spin.)

   (Optional: you may want to think about the more general case $\boldsymbol{p} = (p\sin\theta, 0, p\cos\theta)$.)

   (c) Consider a wave-packet state

$$|\boldsymbol{x}, \boldsymbol{p}\rangle \equiv \mathrm{e}^{-(\hat{\boldsymbol{x}}-\boldsymbol{x})^2/2\xi^2}\psi_{\boldsymbol{p}}$$

   where $|\boldsymbol{p}\rangle$ is the state defined in (a). The particle described by such a state has average position $\boldsymbol{x}$ and average momentum $\boldsymbol{p}$. Use the coherent states $|\boldsymbol{x}, \boldsymbol{p}\rangle$ and the coherent-state approach to obtain a phase-space Lagrangian that determine the classical motion of $\boldsymbol{x}$ and $\boldsymbol{p}$, assuming the potential $V(\boldsymbol{x})$ is almost constant over the scale ξ. Find the equation of motion for $\boldsymbol{x}$ and $\boldsymbol{p}$.

2. (10 pts.) **Electric conductance in graphene**

   The graphene has two Fermi "points" K and K'. The band structure near one Fermi "point" K is described by the $\boldsymbol{k}$-space "hoping matrix"

$$M_K(\boldsymbol{k}) = \hbar v k_x \sigma^x + \hbar v k_y \sigma^y, \tag{1}$$

   where $\boldsymbol{k}$ is measured from the K point, and $\sigma^{x,y,z}$ are Pauli matrices. The band structure near the other Fermi "point" K' is described by the $\boldsymbol{k}$-space "hoping matrix"

$$M_{K'}(\boldsymbol{k}) = \hbar v k_x \sigma^y + \hbar v k_y \sigma^x, \tag{2}$$

   where $\boldsymbol{k}$ is measured from the K' point.

   (a) Assume the chemical potential is $\mu = 0$. Find the density n_e of thermally excited electrons (*ie* the density electrons in the conduction band with positive energy), at temperature T, up to a dimensionless constant. Find the density n_h of thermally excited holes (*ie* the density holes in the valence band with negative energy), at temperature T, up to a dimensionless constant. You will see that $n_e \sim n_h \sim T^2$.

(b) Assuming a temperature independent relaxation time τ. One might expect the conductivity of the graphene is $\sigma \sim n_e \sim T^2$ (as in Drude model). Use the Boltzmann transport equation to find the conductivity of the graphene at temperature T.

3. (20 pts.) **Electric conductance in strained graphene**

Under a certain strain, the band structure of graphene near one Fermi "point" K is described by the $\boldsymbol{k}$-space "hoping matrix"

$$M_K(\boldsymbol{k}) = \hbar v k_x \sigma^x + \hbar v k_y \sigma^y + \Delta\sigma^z, \tag{3}$$

where $\boldsymbol{k}$ is measured from the K point. The band structure near the other Fermi "point" K' is described by the $\boldsymbol{k}$-space "hoping matrix"

$$M_{K'}(\boldsymbol{k}) = \hbar v k_x \sigma^y + \hbar v k_y \sigma^x + \Delta\sigma^z, \tag{4}$$

where $\boldsymbol{k}$ is measured from the K' point.

(a) Find the $\boldsymbol{k}$-space "magnetic" field $\tilde{b}_{xy}$ at K and K' points, for the conduction and the valence bands. Show that the $\boldsymbol{k}$-space "magnetic" field $\tilde{b}_{xy}$ has a peak near K and K' points. What is the total flux carried by the peaks? What is the rough width δk of the peaks? (Hint: you may use Mathematica, Maple, *etc*)

(b) Assume temperature $T = 0$. Also assume the electron density near K-point is n_e^K, and the hole density near K'-point is $n_h^{K'}$. Find the Hall conductivity σ_{xy}^H for small $n_e^K, n_h^{K'}$ limit and large $n_e^K, n_h^{K'}$ limit. Describe qualitatively how the Hall conductivity σ_{xy}^H depends on $n_e^K, n_h^{K'}$.

(c) Consider an electron near the K-point under an electric field $\boldsymbol{E} = E\boldsymbol{x}$. Assume at $t = 0$ the electron has $\boldsymbol{x} = \boldsymbol{k} = 0$. Using the EOM to find the location of electron at time τ. Here we assume τ is small, so that we can treat $\tilde{b}_{xy}$ as $\boldsymbol{k}$ independent. (At time τ we may assume the electron momentum is reset to $\boldsymbol{k} = 0$ due to scattering by impurities. This way we may obtain an average motion of electron under an electric field $\boldsymbol{E}$ and dissipation described by τ.)

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