Phys 507A - Solid State Physics I

Assignment 2: Electronic quasiparticles. *Due Feb. 9th*

1. *Free electron gas in two dimensions.*

   Consider a free electron in two dimensions (energy $\epsilon_k = \frac{\hbar^2 k^2}{2m^*}$).

   (a) Show that the density of states per unit energy and per unit area is given by $\rho(\epsilon) = \rho_0 = \frac{m}{\pi\hbar^2}$. The calculation is identical to the one you did in problem 7 of A1, except that now you have to take spin degeneracy into account.

   (b) The occupation fraction for each state is given by the Fermi-Dirac distribution,

   $$f(\epsilon) = \frac{1}{\mathrm{e}^{\frac{\epsilon-\mu}{k_B T}} + 1}, \tag{1}$$

   where μ is the chemical potential and k_B is Boltzmann's constant. Denote the 2DEG density by $n_{\mathrm{2DEG}} = N/A$, with N the average number of particles and A the area occupied by the electrons. Using this definition, show that the chemical potential depends on temperature according to the expression:

   $$\mu(T) = k_B T \ln\left(\mathrm{e}^{+\frac{n_{\mathrm{2DEG}}}{\rho_0 k_B T}} - 1\right). \tag{2}$$

   (c) The definition of Fermi energy is that it equals the chemical potential at $T = 0$, $\epsilon_F = \mu(T = 0)$. For a 2DEG with $n_{\mathrm{2DEG}} = 10^{11}$ cm^{-2} at $T = 2$ K, calculate the amount by which μ differs from ϵ_F, and the fractional error that you get by assuming $\mu \approx \epsilon_F$ (assume $m^* = m_e$).

2. *Donor impurities in a semiconductor.*

   What makes semiconductors the material of choice in the microelectronics industry is the fact that we can dope them with impurities. Doping controls the amount of charge carriers, hence it controls the semiconductor conductivity.

   Consider the substitution of one of the lattice atoms by another atom with one additional valence electron. For example, for a silicon lattice, substitute one of the silicon atoms by a group V atom (P, As, Sb, Bi). The group V atom is denoted a "donor impurity" because it has valence five, i.e., one electron more than the reference atom Si. In the effective mass approximation (valid for length scales much larger than the lattice spacing), we may assume that this extra electron moves with mass m^*, and sees the group V atom as a Coulomb center with charge $Q = +|e|$ ($e < 0$ is the modulus of the electron's charge). This leads to the effective potential $V(r) = -\frac{\mathrm{e}^2}{4\pi\epsilon_0\epsilon r}$, where the dielectric constant ϵ models the "screening" effect of the silicon medium (the Coulomb force is reduced due to the electronic polarization of the covalent crystal).

(a) Write down the effective Hamiltonian for the extra electron, and find its ground state wavefunction and its ground state energy. Find the effective ionization energy E_d and the effective Bohr radius a^*.

(b) For silicon, assume $\epsilon = 11.7$, and $m^* = 0.3m_e$. Calculate the values of a^* and E_d. Optical ionization experiments show that $E_d \approx 45$ meV. How does our theoretical calculation compare to the measured value?

3. *How to make a two-dimensional electron gas (2DEG).*

A heterojunction is a combination of two semiconductors that forms a two-dimensional electron gas at its interface. Consider a junction of pure AlAs and n-doped GaAs. While AlAs has a similar ("matching") lattice parameter as GaAs, its band gap is much larger. Because of this, carrier electrons in GaAs will not be able to penetrate into AlAs; when we apply an electric field perpendicular to the sample the carrier electrons will be confined at the interface. In this problem, you will find the temperature regime for which these electrons can be considered effectively two-dimensional.

(a) As a simple model, assume the confining potential at the interface is a triangular well: $V(z) = +|e|Ez$ for $z \geq 0$, and $V(z) = \infty$ for $z < 0$. Here $z = 0$ is the interface, and $z > 0$ goes into GaAs. Write down the Hamiltonian for carrier electrons in the effective mass approximation.

(b) Show that the family of wavefunctions

$$\Psi(\boldsymbol{r}) = C_n \mathrm{Ai}(\kappa \mathrm{z} + \xi_\mathrm{n}) \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_\perp}}{\sqrt{\mathrm{A}}}, \tag{3}$$

are eigenstates of the Hamiltonian. Here Ai are Airy functions, and ξ_n are the n-th zeroes of the Airy functions; C_n is a normalization constant (no need to calculate C_n), and $\boldsymbol{r}_\perp = (x, y)$ is the coordinate of the 2D electron. Thus, conclude that the 3D free electron band is now broken into an infinite set of *subbands*, each with dispersion $\epsilon_{n,k} = E_n + \frac{\hbar^2 k_\perp^2}{2m^*}$. Find the subband energy E_n in terms of the confining electric field E. The characteristic length scale $z_0 = 1/\kappa$ gives the "2DEG width". Find z_0 in terms of the confining electric field.

(c) Argue that at low temperatures, $T \ll T_{2D}$, the system will behave like a true 2D electron system. What is the characteristic temperature T_{2D}? Compute the characteristic temperature for a GaAs heterojunction, with confining electric field $E = 10^4$ V/cm (The effective mass for GaAs is $m^* = 0.067m_e$).

4. *Landau levels in the symmetric gauge.*

Consider 2D electrons subject to a magnetic field perpendicular to the plane, $\boldsymbol{B} = B\hat{\boldsymbol{z}}$. In the symmetric gauge, the vector potential equals to $\boldsymbol{A} = \frac{1}{2}\boldsymbol{B} \times \boldsymbol{r} = \frac{B}{2}(-y, x)$ (Note, this is different from the asymmetric gauge $\boldsymbol{A} = Bx\hat{\boldsymbol{y}}$ assumed in the book).

(a) Show that the Hamiltonian for the electrons can be written as

$$\mathcal{H} = -\frac{\hbar^2}{2m^*}\nabla_\perp^2 + \frac{1}{2}m^*\left(\frac{\omega_c}{2}\right)^2 r^2 + \frac{\omega_c}{2}\hat{L}_z, \tag{4}$$

where $\omega_c = \frac{eB}{m^*}$ is the cyclotron frequency, and $\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\theta}$ is the angular momentum operator, with $x = r\cos\theta$ and $y = r\sin\theta$.

(b) The eigenstates of this Hamiltonian are $\Psi_{N,m}(\boldsymbol{r}) = R_{N,m}(r)\mathrm{e}^{im\theta}$, where $N = 0, 1, 2, \ldots$ is a radial quantum number and m is a magnetic quantum number (representing the magnetic moment of the electron going around in a circle). The eigenenergies are $E_{N,m} = \frac{1}{2}(2N + |m| + m + 1)\hbar\omega_c$. Argue that these eigenenergies are identical to the result found for the asymmetric gauge, and find the relationship between the Landau quantum number ν [see Eq. (2.44) in the book] and the quantum numbers N, m.

(c) Consider the wavefunction

$$\Psi_{N=0,m\leq 0}(r,\theta) = r^m \mathrm{e}^{-\frac{r^2}{2l^2}}\mathrm{e}^{im\theta}, \tag{5}$$

for magnetic quantum number $m \leq 0$ only. Here l is the *magnetic length*. Find the value of l such that Eq. (5) is an eigenstate of $\mathcal{H}$ with energy corresponding to the lowest Landau level $\nu = 0$. The magnetic length l sets the scale for magnetic field effects in the 2DEG.
Hint: Use $\nabla_\perp^2\Psi = \frac{1}{r}\partial_r(r\partial_r\Psi) + \frac{1}{r^2}\partial_\theta^2\Psi$.

5. *Semiclassical model of electron dynamics.*

You can think of each electron carrying current in a metal as a wavepacket of Bloch states. If this wave packet has a well defined quasi-momentum (Δk is small), then by the uncertainty principle the wavepacket will run over many unit cells (i.e., $\Delta r \sim 1/\Delta k \gg a$, with a the lattice parameter). In this case we can show that the electron dynamics will be governed by the following equations:

$$\begin{aligned} \dot{\boldsymbol{r}} &= \frac{1}{\hbar}\nabla_{\boldsymbol{k}} E_{n\boldsymbol{k}} \equiv \boldsymbol{v}_{n\boldsymbol{k}}, \\ \hbar\dot{\boldsymbol{k}} &= e\left[\boldsymbol{E}(\boldsymbol{r},t) + \boldsymbol{v}_{n\boldsymbol{k}} \times \boldsymbol{B}(\boldsymbol{r},t)\right], \end{aligned} \tag{6}$$

with the electron charge $e < 0$.

(a) Prove that the wave packet moves in such a way that the electron energy $[E_{nk} + e\phi(\boldsymbol{r}(t))]$ remains constant. *Hint: Compute* $\frac{d}{dt}[E_{nk} + e\phi(\boldsymbol{r}(t))]$ *and use* $\boldsymbol{E} = -\nabla\phi$.

(b) The current density is given by

$$\boldsymbol{J} = \frac{1}{V}\sum_{\text{all electrons}} e\boldsymbol{v} = e\sum_n \int \frac{d^3k}{4\pi^3}\boldsymbol{v}_{nk}\, g_n(\boldsymbol{k}), \tag{7}$$

where $g_n(\boldsymbol{k})$ is a distribution (or occupation) function for each band. A filled band has $g_n(\boldsymbol{k}) = 1$. Prove that the electrical current carried by the electrons of a filled band is always zero. *Hint: Use the theorem that the integral over any primitive cell of the gradient of a periodic function is equal to zero.*

(c) A partially filled band will have $g_n(\boldsymbol{k}) \leq 1$. Prove that the current produced by occupying with electrons a specified set of levels is precisely the same as the current that would be produced if (i) the specified levels were unoccupied and (ii) all other levels in the band were occupied but with charge of $-e$ (opposite to the electron's charge). In other words, we can think of current carriers in a partially filled band as either electrons or holes.

(d) In the absence of an applied electric field, $g_n(\boldsymbol{k}) = f(E_{nk})$ [$f(E_{nk})$ is the Fermi function, as in Eq. (1)]. In this case, prove that $\boldsymbol{J} = 0$ (no current without an electric field).

(e) Under the application of an electric field, the distribution function becomes

$$g_n(\boldsymbol{k}) = f(E_{nk}) + e\boldsymbol{E} \cdot \boldsymbol{v}_{nk}\tau(E_{nk}) \left(-\frac{\partial f(E)}{\partial E} \right), \tag{8}$$

with $\tau(E_{nk})$ the mean free time between collisions for the electron at state $n\boldsymbol{k}$ (also known as the relaxation time). The *conductivity tensor* $\boldsymbol{\sigma}$ is defined from $\boldsymbol{J} = \boldsymbol{\sigma} \cdot \boldsymbol{E}$. Using the equations and definitions above, derive an expression for the tensor $\boldsymbol{\sigma}$ as an integral over d^3k.

(f) Consider an isotropic metal, i.e. with conduction band $E_{nk} = E_{n0} + \frac{\hbar^2 k^2}{2m^*}$. In this case the conductivity tensor will be diagonal, $\boldsymbol{\sigma} = \sigma\mathbf{1}$. Show that the zero temperature ($T = 0$) conductivity is given by

$$\sigma = \frac{ne^2\tau(E_F)}{m^*}, \tag{9}$$

where $n = N/V$ is the carrier electron density (N is the number of electrons in the conduction band).

(g) At $T = 0$, is it correct to say that only electrons at the Fermi level contribute to conductivity? At $T > 0$, which electrons contribute to conductivity?