SFI5711 - Solid State Physics (2020)
List of exercises #3

1. ac conductivity

Consider the Boltzmann equation

$$\frac{\partial f}{\partial t} + \dot{\mathbf{r}} \cdot \nabla_{\mathbf{r}} f + \dot{\mathbf{k}} \cdot \nabla_{\mathbf{k}} f = I[f]$$

for an isotropic electron gas in the presence of a small electric field $\mathbf{E} = \mathbf{E}_0 e^{-i\omega t}$. Recall that, for elastic impurity scattering, $I[f] = I[f_0 + f_1] = -f_1/\tau$. Consider this to be the case and take τ as given. Obtain the real part of the ac conductivity $\sigma(\omega)$ and sketch its behavior as a function of frequency. What is its characteristic frequency scale?

2. Thermoelectric effect

(a) Consider again the Boltzmann equation for an isotropic electron gas where the scattering process is due to elastic impurity scattering. The application of a thermal gradient $\nabla_{\mathbf{r}} T$ (which it is to be considered small) across the sample gives rise to an electric current $\mathbf{J} = \gamma \nabla_{\mathbf{r}} T$. The thermopower S (or Seebeck coefficient) is then given by the ratio $S = -\gamma/\sigma$, and can be measured experimentally. Show that

$$S = -\frac{\pi^2 k_B^2 T}{3e} \left(\frac{\rho'(E_F)}{\rho(E_F)} \right),$$

where $\rho'(E_F)$ is the derivative of the density of states at the Fermi level. [*Hint*: Use the expansion $-\frac{\partial f_0}{\partial E} = \delta(E - E_F) + \frac{\pi^2}{6}(k_B T)^2 \delta''(E - E_F)$, where $\delta''(x)$ is the second derivative of the Dirac delta function defined as $\int g(x)\delta''(x)\,\mathrm{d}x = g''(0)$.]

(b) What does happen for systems in which $\rho(E_F + E) = \rho(E_F - E)$ (for small E, i.e., $E \ll E_F$)? Give an example of a system with such character.

3. Coulomb interaction in graphene

For the electron gas, the dimensionless parameter that controls the relative amplitude of the Coulomb interaction is r_s, where r_s can be tuned by the density of electrons. In graphene, the situation is different. Recall that, due to the linear dispersion near the Dirac points, the Hamiltonian is given by

$$H = -i\hbar v_F \boldsymbol{\sigma} \cdot \sum_j \nabla_{\mathbf{r}_j} + \frac{e^2}{4\pi\epsilon} \sum_{i,j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|},$$

where σ is the vector of Pauli matrices, ϵ is the effective dielectric constant of the system (i.e. graphene sheet plus substract), and $v_F \approx 10^6\,\mathrm{m/s}$ is the Fermi velocity. Show that, for graphene, the dimensionless parameter that controls the relative amplitude of the Coulomb interaction is approximatelly $2.2\epsilon_0/\epsilon$. Therefore, it can be tuned by the substract.

4. Interacting electron gas: perturbation theory

The Hartree-Fock approach can be used to calculate the energy of the interacting electron gas. The same results can be obtained using first-order perturbation theory. In this case, the total energy is given by $E = E_0 + E_1$, where E_0 is the energy of the free electron gas and

$$E_1 = \frac{1}{2V} \sum_{\mathbf{q}\neq 0} \sum_{\mathbf{k},\mathbf{p}} \sum_{\sigma,\tau} V_{\mathbf{q}} \left\langle \mathrm{FS} \left| c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c^\dagger_{\mathbf{p}-\mathbf{q},\tau} c_{\mathbf{p},\tau} c_{\mathbf{k},\sigma} \right| \mathrm{FS} \right\rangle,$$

is the first-order perturbation correction. Here, the average is taken with respect to the ground state of the free electron gas, i.e. the Fermi sea $|\mathrm{FS}\rangle$, the sum excludes the $q = 0$ contribution because it cancels the background of positive charge, V is the volume of the system and $V_{\mathbf{q}} = \frac{e^2}{\epsilon_0 q^2}$ is the usual Coulomb repulsion.

(a) Using the commutation relations of the creation and annihilation operators and the restrictions on the sum in E_1, show that

$$\left\langle \mathrm{FS} \left| c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c^\dagger_{\mathbf{p}-\mathbf{q},\tau} c_{\mathbf{p},\tau} c_{\mathbf{k},\sigma} \right| \mathrm{FS} \right\rangle = -\delta_{\mathbf{k}+\mathbf{q},\mathbf{p}} \delta_{\sigma,\tau} \theta(k_F - |\mathbf{k}+\mathbf{q}|)\,\theta(k_F - k),$$

where $\theta(x)$ is the usual step function and k_F is the Fermi momentum of the free electron gas.

(b) Compute E_1 and express your results as a function of k_F.

(c) Using the definition of the parameter r_s (the ratio between the electronic mean radius and the Bohr radius), show that the total energy is

$$\frac{E}{N} = \left[\frac{2.210}{r_s^2} - \frac{0.916}{r_s}\right] \text{Ry}.$$

Thus, it agrees with the Hartree-Fock calculation. Minimize this energy with respect to r_s and find the optimal value. Is this value small enough to validate perturbation theory?

(d) Consider now second-order corrections

$$E_2 = \sum_{\alpha \neq \text{FS}} \frac{\langle \text{FS}|V|\alpha\rangle \langle \alpha|V|\text{FS}\rangle}{E_{\text{FS}} - E_\alpha}.$$

This is complicate, and thus, focus only on the direct term which corresponds to small momentum transfer. Since $|\alpha\rangle \neq |\text{FS}\rangle$, the direct process involves creating two electrons outside the Fermi surface (with momenta $\mathbf{k}+\mathbf{q}$ and $\mathbf{p}-\mathbf{q}$) and destroying two electrons inside the Fermi surface (with momenta $\mathbf{k}$ and $\mathbf{p}$), such that

$$E_\alpha = E_{\text{FS}} + \frac{\hbar^2}{2m}\left(|\mathbf{k}+\mathbf{q}|^2 + |\mathbf{p}-\mathbf{q}|^2 - k^2 - p^2\right).$$

Therefore,

$$E_2 = \frac{1}{V^2}\sum_{\mathbf{q},\mathbf{k},\mathbf{p}} \frac{V_\mathbf{q}^2}{E_{\text{FS}} - E_\alpha} \theta\left(|\mathbf{k}+\mathbf{q}| - k_F\right)\theta\left(|\mathbf{p}-\mathbf{q}| - k_F\right)\theta\left(k_F - k\right)\theta\left(k_F - p\right).$$

In the limit $q \ll k_F$, show that

$$\sum_{\mathbf{k}} \theta\left(k_F - |\mathbf{k}+\mathbf{q}|\right)\theta\left(k_F - k\right) \propto q, \text{ and } \sum_{\mathbf{p}} \theta\left(k_F - |\mathbf{p}-\mathbf{q}|\right)\theta\left(k_F - p\right) \propto q.$$

By using these expressions, and by expanding $E_{\text{FS}} - E_\alpha$ to leading order in $\mathbf{q}$, show that E_2 diverges logarithmically. (You do not need to evaluate all the integrals, just analyze the behavior of the integration over dq as $q \to 0$.) Therefore, the perturbation series is not convergent. Show that, if we consider a screened Coulomb potential

$$V_\mathbf{q} = \frac{e^2}{\epsilon_0\left(q^2 + k_{\text{TF}}^2\right)},$$

with k_{TF} being a constant, the divergence in E_2 is removed.