



WS14/15 Condensed Matter Physics I
Exercise 4. Electrons II.

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Notice: *In solving the proposed exercises clearly motivate the passages to reach the result. The use of clear and compact notation is greatly encouraged, as well as the systematic use of dimensional checks of the expressions and results. When you are asked to “evaluate” something this means to provide a numerical evaluation of the expression. In this case, at times, it might be necessary to indicate a parameter whose explicit numerical value is not provided, i.e. $\omega_c = 1.76 H$ (Gauss) Hertz. Otherwise specified, all the evaluations are to be given with 3 significant figures.*

4.1 Nearly-free electrons in Dirac-delta potential (10 pts)

Atoms are arranged in one-dimensional chain with lattice spacing a . Each atom is represented by the potential $aV_0\delta(x)$.

1. Assuming that the nearly-free electron approximation applies, calculate the bandgap for all the electronic bands.

[The bandgap opens at the edge of the each Brillouin zone and its value is twice the Fourier component of the potential at that point. Therefore

$$\Delta_G = 2|U_G| = 2 \left| \frac{1}{a} \int_{-a/2}^{a/2} dr aV_0\delta(x)e^{irG} \right| = 2V_0.$$

The bandgap is the same for all the bands.]

2. Consider the band near $k=0$. Using the second order perturbation theory write the expression for the nearly-free electron band.

[Near $k=0$, i.e. far from a Bragg plane, the band dispersion can be obtained by the second order perturbation theory (Ashcroft eq. 9.13)

$$\mathcal{E}(k) = \mathcal{E}_k^0 + \sum_G' \frac{|U_G|^2}{\mathcal{E}_k^0 - \mathcal{E}_{k-G}^0}$$

Here $\mathcal{E}_k^0 = \hbar^2 k^2 / 2m$ is the free electron dispersion. Since the Potential Fourier component are G-independent we get

$$\mathcal{E}(k) = \frac{\hbar^2 k^2}{2m} + \frac{2m}{\hbar^2} V_0^2 \sum_G' \frac{1}{k^2 - (k-G)^2} = \frac{\hbar^2 k^2}{2m} - \frac{2m}{\hbar^2} V_0^2 \sum_n' \frac{1}{G^2 - 2kG}$$

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3. The effective mass of an electron around the gamma point can be written as $\frac{\hbar^2}{m^*} = \left. \frac{\partial^2 E}{\partial k^2} \right|_{k=0}$. By performing the derivative under the sum sign give the expression for the effective mass as a function of the potential parameters.

$$\begin{aligned} \left[\frac{\hbar^2}{m^*} = \frac{\partial^2 E}{\partial k^2} \right]_{k=0} &= \frac{\hbar^2}{m} - \frac{2m}{\hbar^2} V_0^2 \sum_n' \left. \frac{8G^2}{(G^2 - 2kG)^3} \right|_{k=0} = \frac{\hbar^2}{m} - \frac{16m}{\hbar^2} V_0^2 \sum_n' \frac{1}{G^4} \\ &= \frac{\hbar^2}{m} - \frac{2m a^4}{\hbar^2 \pi^4} V_0^2 \sum_n' \frac{1}{n^4} = \frac{\hbar^2}{m} - \frac{2m a^4}{\hbar^2 \pi^4} V_0^2 \frac{\pi^4}{90} = \frac{\hbar^2}{m} - \frac{2m a^4}{\hbar^2 45} V_0^2. \end{aligned}$$

From this we obtain the effective mass:

$$\frac{m^*}{m} = \left[1 - \frac{2m^2 a^4}{\hbar^2 45} V_0^2 \right]^{-1}.$$

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4. Let now $a=a_B$. How large should be V_0 to have $m^*=1.1m_e$? Evaluate V_0 in appropriate units (eV, Ry or Hartree). Is that a strong potential on the atomic scale? What would you compare it with to decide? What happens if the potential changes sign? Comment.

[Considering Hartree units ($e = m = \hbar = 1$) we obtain: $m^* = \left[1 - \frac{2}{45} V_0^2 \right]^{-1}$ Since the variation is small we can approximate to the first order, obtaining $V_0 = 1.5$ Hartree = 40.8 eV. This energy is 3 times the electron binding energy in an Hydrogen atom.

If the potential changes sign the mass remains the same: you can have confinement also with a repulsive potential.

Hint: $\sum_{n=1}^{\infty} n^{-4} = \pi^4/90$.

4.2 Instability of a 1D electron gas

(10 pts)

Consider a one dimensional electron gas, with linear density $n = 1/a$, with a the average spacing between electrons.

1. Evaluate the Fermi energy, Fermi temperature and Fermi momentum and the average energy density of the system as a function of the spacing a .

[For 1D system the Fermi Energy is $E_F = \hbar^2 \pi^2 n^2 / 8m$; this corresponds to a Fermi temperature of $T_F = \hbar^2 \pi^2 n^2 / 8mk_B$.

The Fermi momentum is $k_F = \pi n / 2 = \pi / 2a$. Note that the Fermi momentum is the middle point of the positive half of the FBZ.

The energy density is $nE = (\pi)^{-1} \int_0^{k_F} dk \hbar^2 k^2 / 2m = \hbar^2 k_F^3 / 6m\pi$, $= \frac{\pi n}{6} \hbar^2 k_F^2 / 2m\pi = \frac{n}{6} E_F$ corresponding to an average energy per electron of $\frac{E_F}{6}$.]

2. Consider now a weak periodic potential $V(x) = V_0 \cos(2k_F x)$ applied to the electrons. How many bandgaps it opens and how many bands it creates? Calculate the dispersion $E(k)$ for the lowest energy band.

[To find where the bandgap opens we have to recall the near zone boundary energy dispersion

$$E_{\mathbf{k}} = \frac{1}{2} [E_{\mathbf{k}}^0 + E_{\mathbf{k}+\mathbf{G}}^0] \pm \frac{1}{2} \sqrt{(E_{\mathbf{k}}^0 - E_{\mathbf{k}+\mathbf{G}}^0)^2 + 4V_G^2}$$

(Ashcroft Eq. 9.26 – Lecture 8 slide 19). Here $E_{\mathbf{k}}^0 = \hbar^2 \mathbf{k}^2 / 2m$ is the free electron dispersion. The bandgap opens at a point \mathbf{k} such that $E_{\mathbf{k}}^0 = E_{\mathbf{k}+\mathbf{G}}^0$, i.e. in 1D $\mathbf{k} = \pm(\mathbf{k} + \mathbf{G})$, therefore a bandgap opens for every vector $\mathbf{k} = \pm \mathbf{G} / 2$.

Let us now calculate the Fourier components of the potential. We can see that the potential is periodic over $\frac{2\pi}{2k_F} = 2a$ This corresponds to a doubling of the real space period. i.e. a dimerization. We note that the Wigner-Seitz cell $[-a, a]$ and a FBZ cell $[-\frac{\pi}{2a}, \frac{\pi}{2a}] = [-\frac{G_0}{2}, \frac{G_0}{2}] = [-k_F, k_F]$! We note that FBZ edges is the Fermi surface of the 1D free electron gas and that's where the first bandgap will appear. Therefore the first gap will open at the Fermi energy. This will have fundamental consequence for the stability of the system.

Now the Fourier components of the potential are:

$$\begin{aligned}
V_G &= \frac{V_0}{2a} \int_{-a}^a dx \cos(2k_F x) e^{ixG} = \frac{V_0}{4a} \int_{-a}^a dx [e^{ix(G+2k_F)} + e^{ix(G-2k_F)}] \\
&= \frac{V_0}{2} \left[\frac{\sin a(G+2k_F)}{a(G+2k_F)} + \frac{\sin a(G-2k_F)}{a(G-2k_F)} \right] \\
&= \frac{V_0}{2} [\text{sinc } a(G+2k_F) + \text{sinc } a(G-2k_F)].
\end{aligned}$$

Remembering that the sinc function $\text{sinc } x = \frac{\sin x}{x}$ has a maximum for $x = 0$ we can see that the Fourier amplitude is indeed maximum for $G = \pm 2k_F$. The potential therefore opens a bandgap of about $2V_0$ at $k = k_F$ i.e. at the FBZ edge.]

3. Determine the total energy of the electronic system at zero temperature as a function of V_0 .

[The energy of the gapped system at zero T can be expressed as a sum on the k states, by integrating the energy dispersion

$$E_{\mathbf{k}} = \frac{1}{2} [E_{\mathbf{k}}^0 + E_{\mathbf{k}+\mathbf{G}}^0] \pm \frac{1}{2} \sqrt{(E_{\mathbf{k}}^0 - E_{\mathbf{k}+\mathbf{G}}^0)^2 + 4V_0^2}$$

We are interested on the first energy band, between $[-k_F, k_F]$. This band is given by the formula above, where we have to take $G = +2k_F$ for $k \in [-k_F, 0]$ and $G = -2k_F$ for $k \in [0, k_F]$. Since the band is symmetric we will use only the latter case in the integration below. In Hartree units such dispersion reads:

$$\begin{aligned}
E_{\mathbf{k}} &= \frac{1}{4} [k^2 + (k - 2k_F)^2] - \frac{1}{4} \sqrt{[k^2 - (k - 2k_F)^2]^2 + 16V_0^2} \\
&= \frac{k^2}{2} + k_F^2 - kk_F - \sqrt{[kk_F - k_F^2]^2 + V_0^2} \\
\frac{E[V_0]}{V} &= \frac{1}{V} \sum_k E_k = \frac{1}{2\pi} \int_{-k_F}^{k_F} E_k dk = \frac{1}{\pi} \int_0^{k_F} E_k dk = \\
&= \frac{1}{\pi} \int_0^{k_F} \left[\frac{k^2}{2} + k_F^2 - kk_F - \sqrt{[kk_F - k_F^2]^2 + \frac{V_0^2}{4}} \right] dk \\
&= \frac{2}{3\pi} k_F^3 - \frac{k_F}{2\pi} \sqrt{k_F^4 + V_0^2} + \frac{V_0^2}{2\pi k_F} \log \frac{\sqrt{k_F^4 + V_0^2} - k_F^2}{|V_0|}.
\end{aligned}$$

In the approximation for which $V_0/2k_F^2 \ll 1$ we obtain

$$\begin{aligned}
\frac{E[V_0]}{V} &= \frac{2}{3\pi} k_F^3 - \frac{k_F}{2\pi} \sqrt{1 + \frac{V_0^2}{k_F^4}} + \frac{V_0^2}{2\pi k_F} \log \left[\frac{k_F^2}{|V_0|} \left(\sqrt{1 + \frac{V_0^2}{k_F^4}} - 1 \right) \right] \approx \\
&\approx \frac{2}{3\pi} k_F^3 - \frac{k_F}{2\pi} \left(1 + \frac{V_0^2}{2k_F^4} \right) + \frac{V_0^2}{2\pi k_F} \log \left[\frac{k_F^2}{|V_0|} \left(1 + \frac{V_0^2}{2k_F^4} - 1 \right) \right] = \frac{2}{3\pi} k_F^3 - \frac{1}{2\pi} k_F^3 \\
&\quad - \frac{V_0^2}{4\pi k_F} \left(1 + 2 \log \frac{2k_F^2}{|V_0|} \right) =
\end{aligned}$$

$$= \frac{k_F^3}{6\pi} - \frac{V_0^2}{4\pi k_F} \left(1 + 2 \log \frac{2k_F^2}{|V_0|} \right).$$

Note that for $V_0 = 0$ the energy density is equal to the value for the free Fermi gas found in 1.]

4. For a finite V_0 is the energy change positive or negative? Why is that? What would be the main qualitative different in the case of a 2D or a 3D system? Comment.

[The change is negative for $|V_0| > 0$. This means that for an arbitrarily small dimerization potential the bandgap opening is energetically favoured. This crucially depends on the fact that, for $D=1$, the bandgap opens at the Fermi momentum, therefore the filled states are lowered in energy while the empty states are raised by the bandgap opening.

For $D>1$ the Fermi momentum is not commensurate anymore with a periodicity doubling, therefore the bandgap opening for a dimerization will open a gap either above or below Fermi energy. This will not cause a net energy.

4.3 Conductivity tensor and velocity-velocity correlations (10 pts)

In the Boltzmann theory of electron transport the temperature-dependent conductivity tensor is given by the following general expression

$$\hat{\sigma}_{ij} = -e^2 \int \frac{d\mathbf{k}}{4\pi^3} \left(\frac{\partial f_0}{\partial \epsilon} \right) \tau(\mathbf{k}) v_i(\mathbf{k}) v_j(\mathbf{k})$$

where $f_0(\epsilon, T)$ is the Fermi function and $v_i(\mathbf{k})$ is the i -th component $i, j = (x, y, z)$ of the velocity vector $\mathbf{v}(\mathbf{k})$.

1. Consider a three dimensional electron system at zero temperature in the Drude approximation (i.e. momentum-independent relaxation time). Show that in this case the tensor reduces to

$$\hat{\sigma}_{ij} = \frac{1}{4\pi^3} \frac{e^2 \tau}{\hbar} \int \frac{v_i(\mathbf{k}) v_j(\mathbf{k})}{|v|} dS_F$$

Where the integral is now on the (two dimensional) Fermi surface.

(Hint: use the chain rule to convert the energy derivative into a momentum derivative and remember what happens to the Fermi function in the limit of 0 T...)

[at zero T the Fermi function is a step at Fermi energy. The energy derivative is a delta function: $\frac{\partial f_0}{\partial \epsilon} = \delta(\epsilon_{\mathbf{k}} - \epsilon_F) = \left| \frac{d\epsilon}{d\mathbf{k}} \right|^{-1} \delta(\mathbf{k} - \mathbf{k}_F) = \frac{1}{\hbar|v|} \delta(\mathbf{k} - \mathbf{k}_F)$. We used the basic properties of the delta function and we did explicitly the derivative of the

velocity. The delta function simply means that the only integration is done over the Fermi surface.]

2. Now show that for “free” electrons the conductivity tensor reduces to the Drude expression for the conductivity

$$\sigma = \frac{ne^2\tau}{m}.$$

(Hint: Carefully consider the symmetry of the tensor and of the free electron Fermi surface: you can evaluate most of the $\hat{\sigma}_{ij}$ integrals without explicitly calculating them. You should need to explicitly calculate only a single element of the tensor...)

[In the Drude model the electrons are nearly-free, the Fermi surface is a sphere, the velocity modulus is constant and everything reduces to evaluate the integral over a sphere of the product of the angular components:

$$\hat{\sigma}_{ij} = \frac{v_F}{4\pi^3} \frac{e^2\tau}{\hbar} \int d\Omega \hat{k}_i \hat{k}_j k_F^2.$$

Now, for symmetry reasons the product $\hat{k}_i \hat{k}_j$ is symmetric over inversion for $i \neq j$. Since the integration volume is a sphere the integral vanishes. The only integrals that don't vanish (and are indeed the same) are the one for which $i = j$. In that case

$$\int \hat{k}_z^2 d\Omega = \int_0^{2\pi} d\varphi \int_0^\pi d\theta \sin\theta \cos^2\theta = \frac{4\pi}{3}.$$

By remembering that $v_F = \hbar k_F/m$ and $k_F = (2\pi^2 n)^{1/3}$ the final result is

$$\hat{\sigma}_{ii} = \frac{v_F k_F^2}{4\pi^3} \frac{e^2\tau}{\hbar} \frac{4\pi}{3} = \frac{e^2\tau k_F^3}{3m\pi^2} = \frac{ne^2\tau}{3m}.$$

The total conductivity is simply the Trace of the conductivity tensor:

$$\sigma = \text{Tr}[\hat{\sigma}_{ij}] = 3 \frac{ne^2\tau}{3m} = \frac{ne^2\tau}{m}.$$

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