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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 chian 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.
2. Consider the band near k=0. Using the second order perturbation theory write the expression for the the nearly-free electron band.
3. The effective mass of an electron around the gamma point can be written as $\frac{\hbar^2}{m^*} = \frac{\partial^2 E}{\partial k^2}\Big|_{k=0}$. By performing the derivative under the sum sign give the expression for the effective mass as a function of the potential parameters.
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.

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.
2. Consider now a weak periodic potential $V(x) = V_0 \cos(2k_F x)$ applied to the electrons. How many bangaps it opens and how many bands it creates? Calculate the dispersion $E(k)$for the lowest energy band.
3. Determine the total energy of the electronic system at zero temperature as a function of V_0.
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.

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

In the Boltmann theory of electron transport the temperature-dependnet 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
$$\hat{\sigma}_{ij} = \frac{1}{4\pi^3} \frac{e^2 \tau}{\hbar} \int \frac{v_i(\mathbf{k})\, v_j(\mathbf{k})}{v} dS_{\mathrm{F}}$$
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…)
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…)