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WS16/17 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.

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 Current in a Landau Level (10 pts)

Let us consider 2D free electron in a magnetic field B. In the Landau Gauge the vector potential is $\mathbf{A} = (0, Bx)$. The Hamiltonian is

$$H = \frac{\hbar^2}{2m}\left[-\frac{\partial^2}{\partial x^2} + \left(-i\frac{\partial}{\partial y} + \frac{x}{\ell^2}\right)^2\right],$$

Where $\ell = \sqrt{\hbar c/eB}$. Note that the component of the velocity operator are $v_x = -\frac{i\hbar}{m}\frac{\partial}{\partial x}$ and $v_y = \frac{\hbar}{m}\left(-i\frac{\partial}{\partial y} + \frac{x}{\ell^2}\right)$. The levels for this Hamiltonian are discreet and the eigenfunctions at the lowest level can be chosen as

$$\psi_k(x,y) = e^{iky}\chi(x + \ell^2 k), \qquad \chi(x) = \left(\frac{1}{\pi\ell^2}\right)^{1/4} e^{-x^2/2\ell^2},$$

where k is a real number. The $\chi(x)$ is normalized over $(-\infty, \infty)$.

1. Calculate the current on the generic state k, disregarding the normalization:

   $j_x(x,y) \propto \psi_k^*(x,y)v_x\psi_k(x,y) + c.c.$ and $j_y(x,y) \propto \psi_k^*(x,y)v_y\psi_k(x,y) + c.c.$

2. Impose now periodic boundary condition along y: $\psi_k(x,y) = \psi_k(x,y+L)$. This allows only some values of k to be admissible. Which ones? Write the generic wavefunction normalized over the appropriate cell.
3. Let us now consider non interacting electrons occupying all the allowed k´s. Obtain the density

   $$n(x,y) = \sum_{k\ allowed} |\psi_k(x,y)|^2.$$

   How this density depends from the y direction? Is the density n periodic along x? with which period?

4.3 Degenerate semiconductor (10 pts)

Consider a semiconductor for which the non-degeneracy condition is not verified. In other words you **cannot** assume $\epsilon_c - \mu \gg K_B T$ and $\mu - \epsilon_c \gg K_B T$. However, for this semiconductor the following relation

$$g_v(\epsilon) = g_c(-[\epsilon - E_0] + E_0)$$

holds. Here $g_v(\epsilon)\ and\ g_c(\epsilon)$ are the DOS of the valence and conduction bands and $2E_0 = \epsilon_c + \epsilon_c$. Moreover it is possible to neglect the impurity (intrinsic regime).

1. Assume that the top of the conduction band is at the energy $\epsilon_c + 2\Delta$. Draw a qualitative drawing of the density of states $g_c(\epsilon)$, paying attention to its behavior at

the two band extrema. In particular specify the qualitative behavior of the DOS at those points.

2. By making use of the above-written relation, draw on the same graph $g_c(\epsilon)$ and $g_v(\epsilon)$.
3. Write the condition that determines the chemical potential and, by rearranging in a simple way one of the integrals, determine the chemical potential μ at every temperature. *[Note: no explicit integration is needed! Moreover, put the energy zero at the half of the gap, in such a way that* $2E_0 = \epsilon_c + \epsilon_c = 0$*.]*
4. Consider now a density of states of the form $g_c(\epsilon) = A\sqrt{(\epsilon - \epsilon_c)(2\Delta - \epsilon + \epsilon_c)}$. Determine the constant A in terms of the density of lattice sites n_L and Δ.
5. Express the effective mass at the bottom of the conduction band in terms of n_L and Δ. Knowing that $n_L = 5.00 \times 10^{22}\ cm^{-3}$ and that $\Delta = 27.7$ eV evaluate the ratio m_c/m_e.

Note: $\int dx\sqrt{1-x^2} = \left[x\sqrt{1-x^2} + arcsin\, x\right]/2$.