PHY 491 - 2013

Atomic, Molecular, and Condensed Matter Physics

Problem Set 10

1. Show that, for a smooth function $f(x)$ and for $\Delta \to 0$,

$$\int_{E-\frac{1}{2}\Delta<f(x)<E+\frac{1}{2}\Delta} dx = \Delta \cdot \int dx \delta\Big(E - f(x)\Big)$$

   Also use the definition of an integral to show that, for $k = m/L$ with integer m and for a smooth function $f(k)$, in the limit of large L

$$\sum_m f(k) = L \int dk f(k)$$

   Indicate the limits of the sum and the integral (5 pt)

2. Consider Born-von Karman periodic boundary conditions, with the periods along the primitive lattice vectors $\mathbf{a}_1, \mathbf{a}_2$, and $\mathbf{a}_3$ being N_1, N_2, and N_3, respectively; $N_{1,2,3}$ are integers, $N_{1,2,3} \gg 1$. Specify the discrete values $\mathbf{k_m}$ of the wave vectors $\mathbf{k}$ for plane waves in the system (the integer-valued vector $\mathbf{m} = (m_1, m_2, m_3)$ enumerates the values of $\mathbf{k}$). Consider a Fourier component of a periodic smooth function $f(\mathbf{r}) = f(\mathbf{r} + N_i\mathbf{a}_i)$ for $\mathbf{k} = \mathbf{k_m}$,

$$f_{\mathbf{k}} = \int_\Omega d\mathbf{r} e^{i\mathbf{kr}} f(\mathbf{r})$$

   Here, region Ω corresponds to the bulk of the crystal, with volume $N_1 N_2 N_3 |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|$. Derive the expression for $f(\mathbf{r})$ in terms of $f_{\mathbf{k}}$. (5 pt)

3. Relate the perturbation theory for coefficients $c_{\mathbf{k}-\mathbf{K}}$ used in class and in the textbook (Chapter 9) to calculate the electron energy in a weak periodic potential away from resonances $\mathcal{E}^{(0)}(\mathbf{k}) = \mathcal{E}^{(0)}(\mathbf{k} + \mathbf{K})$ to the perturbation theory you used in quantum mechanics for a system with Hamiltonian $H = H_0 + \epsilon H_1$ for $\epsilon \ll 1$. Indicate the relation between the wave functions in these formulations (3 pt)

4. Calculate the energy spectrum for a one-dimensional electron system in a weak periodic potential $U(x) = U(x + a)$. Use that $\mathcal{E}^{(0)}(\mathbf{k}) \approx \mathcal{E}^{(0)}(\mathbf{K}/2) + \mathbf{v} \cdot (\mathbf{k} - \mathbf{K}/2)$ for small $|\mathbf{k} - \mathbf{K}/2|$ and $K = 2\pi/a$. Find $\mathbf{v}$. Find the density of levels for energies $E < \hbar^2(\pi/a)^2/m_e$. Keep U_K-dependent terms only where they are not small compared to other terms in the energy. (7 pt)

You are supposed to get 20 points. The solution is due on November 13.