MATERIALS PHYSICS II FALL 2007 HOMEWORK PROBLEMS 7

Return to Robert (mailbox Physics 2nd floor) by Tuesday 30.10.2007 at noon.

Comment: working through the weekly problems as team work is completely acceptable and even recommended, as far as each person writes down and returns his/her own solutions!

1. We investigate the validity of periodic boundary conditions for a one-dimensional free electron gas of N noninteracting electrons. We do this by considering two cases. We first consider a periodic system (P) with normalized eigenfunctions

$$\phi_n(x) = \frac{1}{\sqrt{L}} e^{\frac{2\pi n x i}{L}}$$

and eigenenergies

$$\epsilon_n = \frac{\hbar^2}{2m}(\frac{2\pi n}{L})^2$$

satisfying periodic boundary conditions $\phi(0) = \phi(L)$. Then we consider the same number of electrons in a box (B) with hard wall boundary conditions $\phi(0) = \phi_(L) = 0$. In this case the normalized eigenfunctions are given by

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin(\frac{n\pi}{L})$$

with eigenenergies

$$\epsilon_n = \frac{\hbar^2}{2m}(\frac{\pi n}{L})^2$$

We further assume the system to be spincompensated (i.e. as many up as down spin electrons)

a) What are the degeneracies of the levels of the periodic system P and and the box system B ?

b) Calculate the total energies E_P and E_B of both systems with the same number of particles N. Show that $E_B > E_P$ but that

$$\lim_{N\to\infty} \frac{E_P}{E_B} = 1$$

c) Calculate the electron density $n_P(x)$ and $n_B(x)$ of both systems and show that (except for $x = 0, L$ where $n_B(0) = n_B(L) = 0$)

$$\lim_{N\to\infty} \frac{n_B(x)}{n_P(x)} = 1$$

To answer these questions you may find one or more of the following formulas useful

$$\sum_{n=1}^{M} n^2 = \frac{1}{6}M(M+1)(2M+1) \quad (1)$$

$$\sum_{n=-M}^{M} e^{i\theta n} = \frac{\sin((2M+1)\frac{\theta}{2})}{\sin\frac{\theta}{2}} \quad (2)$$

(5 points)

2. We now study some properties of large but finite crystals and see how the Bloch functions are obtained in the limit of the infinite crystal. For simplicity we consider a one-dimensional case. Consider a particle described by the Schrödinger equation (in atomic units)

$$(-\frac{1}{2}\frac{d^2}{dx^2} + V(x))\psi(x) = \epsilon\psi(x)$$

We now study the Fourier coefficients $c(k)$ of $\psi(x)$ defined by

$$\psi(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, c(k)\, e^{-ikx}$$

a) Show that the Fourier coefficients satisfy the equation

$$\frac{p^2}{2}\, c(p) + \int_{-\infty}^{+\infty} \frac{dq}{2\pi}\, \tilde{V}(q) c(p-q) = \epsilon\, c(p)$$

where $\tilde{V}(q)$ are the Fourier coefficients of $V(x)$.
b) We now consider a finite crystal and let $V(x)$ be of the form

$$V(x) = \sum_{n=-M}^{M} v(x - na)$$

where $v(x)$ are localized potentials and a is a lattice constant.
c) Show that

$$\tilde{V}(q) = \tilde{v}(q)\Delta_M(q)$$

where we defined

$$\Delta_M(q) = \frac{\sin((2M+1)\frac{qa}{2})}{\sin(\frac{qa}{2})}$$

(you can use useful formula (2) of question (1))
d) Show that for large M the function $\Delta_M(q)$ starts behaving like a periodic array of delta-functions with peaks becomes infinitely large when $M \to \infty$ whereas the volume under each peak becoming equal to $2\pi/a$ (to show the latter it will be useful to use formula (2) of question (1))
e) Show that for $M \to \infty$ the equation for the Fourier coefficients $c(p)$ becomes

$$\frac{p^2}{2}\, c(p) + \sum_{j=-\infty}^{\infty} \frac{1}{a}\tilde{v}(G_j) c(p - G_j) = \epsilon\, c(p)$$

where we defined $G_j = 2\pi j/a$.
f) Show that in this case the wavefunction $\psi(x)$ will attain a Bloch form, i.e. be product of a plane wave times a periodic function.

g) For large but finite values of M we do not have translational symmetry. What happens to the Fourier coefficients $c(p)$ in this limit? Will we still have a band structure in this case ? Show that if $c(p)$ are smooth functions of p then $\psi(x)$ will go to zero if x is large enough. How large needs x to be if we want to make $\psi(x)$ small (this can be answered semi-qualitatively)
(5 points)