Introduction to Condensed Matter
PHY 251/PHY 420

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— ASSIGNMENT 3, 11/7/2011 — Due 11/14/2011

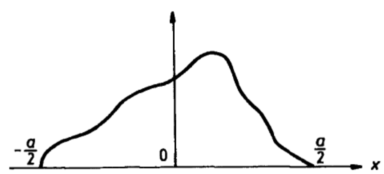
(*Undergraduate students do not have to answer the questions marked with the symbol* ■.)

1 Electron Tunneling and Energy Bands *(35 points)*

(*Hint*: Read Problem 1, pag. 146, N. W. Ashcroft and N. D. Mermin, *Solid State Physics*, Brooks Cole (1976).)
A one-dimensional periodic potential $V(x)$ is formed by superposition of identical potential barriers $v(x)$ of width a, centered at the points $x = \pm na$, where n is an integer,

$$V(x) = \sum_{n=-\infty}^{+\infty} v(x - na).$$

The barrier $v(x)$, schematically drawn in Fig. 1, may be characterized by a transmission coefficient $t(k)$ and a reflection coefficient $r(k)$ for an electron incident on the barrier with a certain energy.



(a) For the single barrier case, write down the most general solution for the wave function of an electron with energy E such that $2mE = \hbar^2 k^2$.

(b) Imposing the Bloch condition at $x = -a/2$, how is the kinetic energy of the Bloch electron ($2m(E - V) = \hbar^2 \kappa^2$, with κ the crystal momentum) related to its wave vector k for the total crystal potential $V(x)$. How does this relation simply for symmetric potential ($v(x) = v(-x)$)? Verify that this gives the right answer in the free-electron case $V = 0$.

(c ■) By recalling some simple properties of t and r, demonstrate that Bloch waves occur only in bands of energies.

(d ■) Suppose the barriers are weak, i.e., $|t| \approx 1$ and $|r| \approx 0$, find a simple expression for the width of the energy gaps.

2 Examples of Crystal Potentials *(45 points)*

An electron in one-dimension is subject to the potential (with $V_1 > 0$)

$$V(x) = 2V_1[1 - \cos(\frac{2\pi x}{a})].$$

(a) Derive the corresponding central equation for the coefficients C_k and write down the generic 5×5 block of the corresponding determinant (see pag. 174, C. Kittel, *Introduction to Solid State Physics*, Wiley; 8th ed. (2005)).

(b) Assuming weak potential, i.e., small V_1, apply stationary perturbation theory (nearly free electron approximation) to solve for $k = 0$ and $k = \pi/a$.

Consider now the electron to be in a two-dimensional square lattice with crystal potential

$$V(x, y) = -4V_1 \cos(\frac{2\pi x}{a}) \cos(\frac{2\pi y}{a})$$

(c) Assuming small V_1 like in (b), solve the central equation to find approximately the energy gap at the corner points $(\pi/a, \pi/a)$ of the first Brillouin zone. (It will suffice to solve a 2×2 determinantal equation.)

3 General Properties of the Bloch Electrons *(20 points)*

The Bloch theorem allows us to make general statements about the eigenstates of the Bloch electrons even without knowing anything about the periodic potential form in a particular crystal. With $\vec{G}$ a reciprocal lattice vector, demonstrate that

(a)

$$\psi_{n,\vec{k}+\vec{G}}(\vec{r}) = \psi_{n,\vec{k}}(\vec{r}); \quad E_{n,\vec{k}+\vec{G}} = E_{n,\vec{k}}$$

(b)

$$\psi^*_{n,\vec{k}}(\vec{r}) = \psi_{n,-\vec{k}}(\vec{r}); \quad E_{n,-\vec{k}} = E_{n,\vec{k}}$$

(c ■) Demonstrate that the electron bands at the zone boundaries have either a maximum or a minimum in the direction normal to the boundary,

$$\frac{\partial}{\partial k} E_{n,\vec{k}} \bigg|_{\vec{k}=\vec{G}/2} = 0,$$

and for every direction

$$\nabla_{\vec{k}} E_{n,\vec{k}} \bigg|_{\vec{k}=0} = 0.$$