Solid State Theory

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Sheet 7: return on: Monday, Jan 21, 2013, 12:00 (SR THP)

Exercise 1: Bloch factors; inversion symmetry

In the lectures, perturbation theory was used to derive the effective mass of an electron from the differential equation for the Bloch factors (see section 4.3 of the script).

a) Following the notation of the script, show that if the potential V is an even function of $\vec{r}$, (i.e. $V(\vec{r}) = V(-\vec{r})$), than also $v_{n\vec{0}}$ is an even function of $\vec{r}$. Explain how you use the fact that the spectrum of $h(\vec{0})$ is non degenerate. (2 points)

b) Use this fact to show that $\langle n^{(0)}|\vec{k}\cdot\vec{p}|n^{(0)}\rangle$. Note that $\langle\vec{r}|n^{(0)}\rangle = v_{n\vec{0}}(\vec{r})$. (2 points)

Exercise 2: Tight-binding model

In this exercise we will use the tight-binding model to analyse the following system. Consider a one dimensional chain of ions, with lattice spacing a, each to which one electron is attached. The potential fields of the ions is to be modelled by a delta-peak. Thus we have a potential $V(x) = -v_0 \sum_{n\in\mathbb{Z}} \delta(x - na)$.

a) First calculate a single electron wave function in the potential of a single ion. Thus in other words, solve the following Schrödinger equation:

$$-\frac{\hbar^2}{2m}\phi''(x) - v_0\delta(x)\phi(x) = E_0\phi(x) \tag{1}$$

Hint: Use $\kappa = \frac{mv_0}{\hbar^2}$ to simplify your expression. Or use another symbol if your handwritting doesn't allow to use both κ and k. (3 points)

b) Give a handwaving argument why it is a good approximation to only correct for overlap between nearest neighbor electron wavefunctions. (2 points)

c) Only using nearest neighbor interactions, the energy spectrum according to the tight-binding model becomes:

$$E(k) = E_0 + \frac{\beta + 2\cos(ka)\lambda}{1 + 2\cos(ka)\alpha} \tag{2}$$

where β, λ and α are wavefunction overlaps defined by:

$$\beta = \int dx \phi(x) \left[V(x) - v(x) \right] \phi(x) \tag{3}$$

$$\lambda = \int dx \phi(x-a) v(x-a) \phi(x) \tag{4}$$

$$\alpha = \int dx \phi(x-a) \phi(x) \tag{5}$$

and $v(x)$ the potential of a single ion located at site x. Calculate β, λ and α for our model. (4 points)

d) Calculate $E(k)$. Keep only the leading order terms of $e^{-\kappa a}$. (2 points)

Exercise 3: Fermi surface

a) Consider a square lattice with lattice spacing a. Use the tight-binding approximation as defined by equations 4.81 - 4.84 in the book of G. Czycholl (Theoretische Festkörperphysik) to calculate the energy spectrum. Assume that the wavefunction overlaps behave as: $\lambda(R) \propto e^{-cR}$, $\beta \propto e^{-2ca}$, $\alpha(R) \propto e^{-cR}$, where c is some constant. Keep only leading order terms in $e^{-ca} := t$. (3 points)

b) Give the Fermi surface for Fermi energies $E_F = -t, 0$ or t. (2 points)