Quantum theory of condensed matter I

PD Dr. Andrea Donarini
Dr. Ivan Dmitriev

PD Dr. Andrea Donarini	Tue	10:00 - 12:00	H33
	Thu	10:00 - 12:00	H33
Dr. Ivan Dmitriev	Tue	12:00 - 14:00	9.2.01

Sheet 5

1. Nearly free electron Fermi surface near a single Bragg plane

Let us consider the nearly free electron band structure close to a single Bragg plane:

$$\epsilon_{\pm}(\mathbf{q}) = \frac{\epsilon^0_{\mathbf{q}} + \epsilon^0_{\mathbf{q}-\mathbf{G}}}{2} \pm \sqrt{\left(\frac{\epsilon^0_{\mathbf{q}} - \epsilon^0_{\mathbf{q}-\mathbf{G}}}{2}\right)^2 + \left|\tilde{V}(\mathbf{G})\right|^2} \tag{1}$$

1. Prove that, if we write $\mathbf{q} = \frac{1}{2}\mathbf{G} + \mathbf{k}$ and resolve $\mathbf{k}$ into its components parallel ($k_{||}$) and perpendicular ($k_{\perp}$) to the Bravais lattice vector $\mathbf{G}$, the dispersion relation for the two bands given in Eq. (1) becomes:

$$\epsilon_{\pm}(\mathbf{k}) = \epsilon^0_{\mathbf{G/2}} + \frac{\hbar^2}{2m}k^2 \pm \sqrt{4\epsilon^0_{\mathbf{G/2}}\frac{\hbar^2}{2m}k^2_{||} + \left|\tilde{V}(\mathbf{G})\right|^2}$$

(1 Point)

Consider now an electronic density which corresponds to a Fermi energy $\epsilon_F = \epsilon^0_{\mathbf{G/2}} - |\tilde{V}(\mathbf{G})| + \Delta$.

2. Show that when $0 < \Delta < 2|\tilde{V}(\mathbf{G})|$, the Fermi surface lies entirely in the lower band and intersects the Bragg plane in a circle of radious:

$$\rho = \sqrt{\frac{2m\Delta}{\hbar}}.$$

(2 Points)

3. Show that if $\Delta > 2|\tilde{V}(\mathbf{G})|$, the Fermi surface lies in Both bands, cutting the Bragg plane in two circles of radii ρ_1 and ρ_2 and that the difference in the area of the two circles is:

$$\pi(\rho_2^2 - \rho_1^2) = \frac{4m\pi}{\hbar^2}|\tilde{V}(\mathbf{G})|.$$

(2 Points)

2. Density of states for tight binding models

Consider the following tight-binding Hamiltonian representing the valence electrons of an infinite chain of atoms with the lattice constant a:

$$\hat{H} = \lim_{N_{\text{sites}}\to\infty} -t \sum_{i=1}^{N_{\text{sites}}} \left(|i\rangle\langle i+1| + |i+1\rangle\langle i|\right),$$

where for simplicity the spin is neglected and we assume periodic boundary conditions.

1. Prove that the density of states for the system reads (in the limit $N_{\text{sites}} \to \infty$)

$$\rho(E) = \frac{1}{\pi} \frac{1}{\sqrt{4t^2 - E^2}}$$

for $|E| < 2t$ and vanishes elsewhere. Hint: start from the definition of the density of states,

$$\rho(E) = \frac{1}{N_{\text{tot}}} \sum_{\alpha} \delta(E - E_{\alpha}),$$

where N_{tot} is the total number of states for the system and α is labelling the eigenstates of the system with eigenvalue E_{α}. The following relation involving the Dirac delta can be useful:

$$\delta(f(x)) = \sum_i \frac{1}{|f'(x_i)|} \delta(x - x_i),$$

where the points x_i are the zeroes of $f(x)$. **(2 Points)**

2. What is the density of states for a 1-dimensional free electron gas? Compare it with the result calculated in the previous point. **(2 Points)**

3. Now consider the generalization of the tight-binding model of an infinite chain to a square (2D) and a cubic (3D) lattice. What are the dispersion relations in these two cases? **(1 Point)**

4. **(Oral)** Prove that the density of states can be reduced to the generic form

$$\rho_d(E) = \frac{1}{\pi} \int_0^{\infty} d\lambda \, \cos(\lambda E) \, J_0^d(2t\lambda), \tag{2}$$

where $J_0(x)$ is a Bessel function defined as

$$J_0(x) = \frac{1}{\pi} \int_0^{\pi} dy \, \exp(-ix \cos y)$$

and d is the dimensionality, $d = 1, 2, 3$. Argue from Eq. (2) that the Fermi energy of chain, square or cubic lattice crystal of monovalent atoms it is always vanishing.

Hint: the following relations may be useful

$$\begin{aligned} \delta(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dy \, e^{-ixy}, \\ J_0(-x) &= J_0^*(x) = J_0(x). \end{aligned}$$

Frohes Schaffen!