Quantum Theory of Condensed Matter

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Room H33
Wednesdays at 13:15

Sheet 7

1. Fermi surface of a 2D lattice

Consider a free electron gas in a quadratic lattice with lattice constant a:

1. Construct the first 3 Brillouin zones (BZ's) of the quadratic lattice.
2. Draw the free Fermi "line"circles corresponding to the Fermi wave vectors $k_F = 1.2\pi/a$ and $k_F = 1.65\pi/a$.
3. Draw the Fermi surface in the reduced zone scheme, by folding back the parts of the Fermi surface which fall into the 2nd and 3rd Brillouin zones into the 1st BZ.
4. For these two Fermi wave vectors, draw the corresponding "pockets" of occupied electron states in the first 3 bands in the repeated zone scheme.
5. How are the Fermi lines affected by a weak periodic potential (make just a qualitative sketch)?

2. Density of states for tight binding models

Consider the following tight binding Hamiltonian representing the valence electrons of an infinite chain of atoms at distance a:

$$H = \lim_{N\to\infty} -t \sum_{i=1}^{N} (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i)$$

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

1. Diagonalize the Hamiltonian.
2. Prove that the density of states for the system reads (in the limit $N \to \infty$):

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

   for $|E| < 2t$ and vanishes elsewhere.

   Hint: Start from the definition of the density of states:

   $$\rho(E) = \frac{1}{N} \sum_{\alpha} \delta(E - E_\alpha)$$

   where N 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 distribution function can be useful:

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

   where x_i are all the points such that $f(x_i) = 0$

3. What is the density of states for a 1-dimensional free electron gas? What does it have in common with the result calculated at point 2.2 ?

4. Now consider the generalization of the tight binding model of point 2.1 to a square lattice (2D) and cubic lattice (3D). Which are the dispersion relations in this two cases?

5. Prove that the density of states can be reduced to the generic form:

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

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

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

   and d is the dimensionality $d = 1, 2, 3$. Hint: The following relations can be useful:

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

6. Prove that the density of states for the 1-dimensional tight binding model obtained at point 2.5 and 2.2 coincides.

Frohes Schaffen!