Exercise for Theoretical Condensed Matter Physics

Exercise 1, April, 4th 2024. Discussion on April, 15th 2024

1) The tight-binding Hamiltonian in second quatization in 1D and 2D

In some crystals the valence electrons can be tightly bound to their host ions. A good starting point for analyzing such systems is to describe the kinetic energy by hopping processes, where with the probability amplitude t one valence electron can hop from an ion j to one of the nearest neighbor ions $j + \delta$ (as usual $\{c_j^\dagger, c_{j'} = \delta_{j,j'}\}$):

$$H = -t \sum_{j,\delta} c_{j+\delta}^\dagger c_j, \tag{1}$$

This Hamiltonian is known as the tight-binding Hamiltonian.

a) Consider a 1D lattice with N sites, periodic boundary conditions, and a lattice constant a. Here $j = 1, 2, \ldots, N$ and $\delta = \pm 1$. Use the discrete Fourier transformation $c_j = (1/\sqrt{N}) \sum_k e^{ikja} c_k$ to diagonalize H in k-space and plot the eigenvalues ε_k as a function of k.

b) In high-temperature superconductors the conduction electrons are confined to parallel CuO-planes, where the ions form a 2D square lattice. In this case the 2D tight-binding model is applicable. Generalize the 1D model to a 2D square lattice also with the lattice constant a and plot contours of constant energy $\varepsilon_{k_x k_y}$ in the $k_x k_y$ plane.

c) In many-body theory the excitation energy is defined as as the difference between the energies of a state with $N + 1$ particles and a state with N particles. Show that in the case of model under consideration $\varepsilon_{\mathbf{k}}$ are the excitation energies. Discuss the role of the chemical potential. What chemical potential is implied in the model (1)? To which physical system does it correspond?

Suggestion: Solve tasks 1a and 1b analytically and plot also the band structures using e.g. Python and Matplotlib.