

Quantum Theory of Condensed Matter I

Prof. Milena Grifoni
 Dr. Andrea Donarini
 Sebastian Pfaller

5.1.01 Mondays 10:15
 9.2.01 Tuesdays 12:15

Sheet 12

1. Open questions

Give a concise (and as much as possible precise) answer to the following questions:

- Explain the presence of continuous energy bands in the spectrum of a solid, if compared with the discrete energy spectrum of an atom. **(2 Points)**
- Electron-electron interaction can be considered as a perturbation at high electron densities. Substantiate this counterintuitive statement. **(2 Points)**
- Define the concept of phonon. Compare the Einstein and the Debye models for the calculation of the specific heat at constant volume for a solid. **(2 Points)**

2. Density of states of an infinite ribbon

Let's us consider an infinite ribbon made of N_y chains of atoms organized in a square lattice (see Fig. 1). The valence (spinless) electrons are described by the tight binding Hamiltonian:

$$H = \lim_{N_x \rightarrow \infty} t \sum_{\langle i,j \rangle} c_i^\dagger c_j \quad (1)$$

where the sum runs over nearest neighbors and we assume periodic boundary conditions in the x direction (*i.e.* $N_x + 1 = 1$).

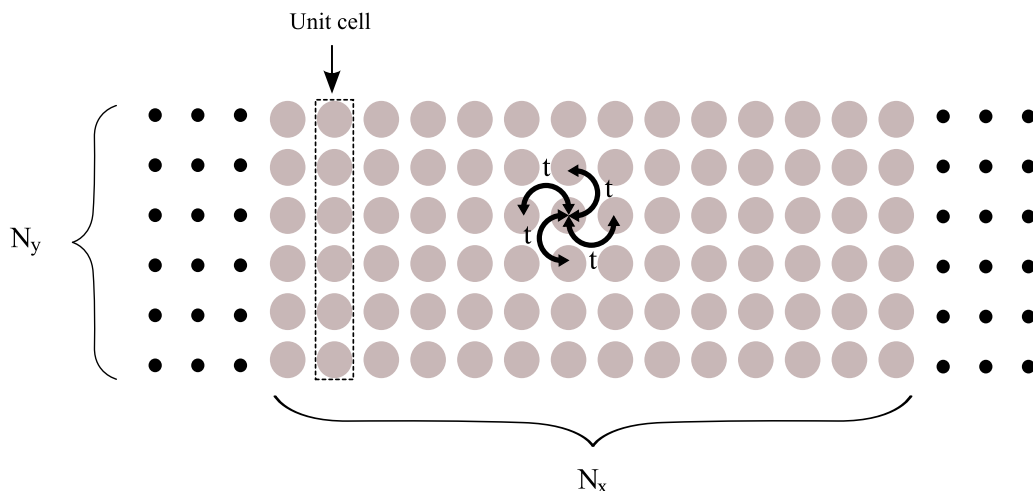


Fig. 1

1. The ribbon is invariant under translation in the x direction by any multiple of lattice unit. Use the Bloch theorem to block diagonalize the Hamiltonian for $N_x \rightarrow \infty$ and calculate the band structure for the ribbon for the case with $N_y = 2, 3$. How many bands do you obtain in each case? **(3 Points)**

2. Consider now the isolated unit cell (see figure). Call ϵ_n and $|n, R\rangle$, $n = 1, \dots, N_y$ the eigenenergies and eigenstates of the unit cell in position R , respectively. Prove that the ribbon hamiltonian (1) is equivalent to the Hamiltonian of N_y independent chains of atoms where the n -th chain is characterized by an on-site energy ϵ_n and the same hopping t of the ribbon, *i.e.*:

$$H = \sum_{n=1}^{N_y} \left(\sum_R \epsilon_n |n, R\rangle \langle n, R| + t |n, R\rangle \langle n, R+a| + t |n, R+a\rangle \langle n, R| \right) \quad (2)$$

Hint: the n -th eigenstate of an open chain of N atoms reads:

$$|n\rangle = \left(\frac{2}{N+1} \right)^{1/2} \sum_{\alpha=1}^N \sin \left(\frac{\pi}{N+1} n \alpha \right) |\alpha\rangle$$

(4 Points)

3. Prove that the density of states (normalized to the length) of the ribbon reads:

$$\rho(E) \equiv \lim_{N_x \rightarrow \infty} \frac{1}{N_x} \sum_{\alpha} \delta(E - \epsilon_{\alpha}) = \sum_{n=1}^{N_y} \frac{1}{\pi \sqrt{4t^2 - (E - 2t \cos(\pi/(N_y + 1)n))^2}}$$

where α is a collection of quantum numbers labeling the eigenstates of the ribbon.

(2 Points)

Frohes Schaffen!