

Freie Universität Berlin  
Tutorials for Advanced Quantum Mechanics  
Wintersemester 2018/19  
Sheet 6

Due date: 10:15 30/11/2018

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1. **Electrons with a Coulomb interaction in the atomic limit** (5×3 points)

In lectures you investigated the Hamiltonian of electrons with a Coulomb interaction in the thermodynamic limit. Now we will consider the same problem in a somewhat different limit, sometimes called the atomic limit. In this limit (see Fig. 1) we imagine a lattice of atoms widely separated by a distance  $a$ . The idea is that this situation should be close to the non-interacting case (i.e. essentially isolated atoms). By writing out the interacting problem in a basis of orbitals localised around the  $N$  lattice points, we can identify terms that should be small and construct an effective Hamiltonian for this limit.

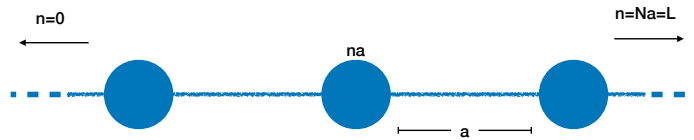


Figure 1:  $N$  atoms in one spatial dimension separated by a distance  $a$  arranged over a length  $L$  with periodic boundary conditions (i.e. on a ring). The smallest case that makes sense is therefore  $N = 3$ .

The Hamiltonian is given by,

$$\hat{H} = \hat{H}^{(0)} + \frac{1}{2} \int dx \int dx' \sum_{\sigma\sigma'} c_{\sigma}^{\dagger}(x) c_{\sigma'}^{\dagger}(x') \frac{e^2}{|x-x'|} c_{\sigma'}(x') c_{\sigma}(x) \quad (1)$$

where

$$\hat{H}^{(0)} = \int dx \sum_{\sigma} c_{\sigma}^{\dagger}(x) \left[ \frac{\hat{p}^2}{2m} + V(x) \right] c_{\sigma}(x) \quad (2)$$

is the non-interacting Hamiltonian for electrons in a periodic potential (i.e. simply interacting with the background ions but not with each other) and the second term is the Coulomb interaction.

- (a) *Make a phenomenological argument for why the effective Hamiltonian in this widely separated limit should turn out to be of the form,*

$$\hat{H} = -t \sum_{\langle mn \rangle} \sum_{\sigma} c_{m\sigma}^{\dagger} c_{n\sigma} + U \sum_m \hat{n}_{m\uparrow} \hat{n}_{m\downarrow} \quad (3)$$

where the operators  $c_{m\sigma}^{\dagger}$ ,  $c_{m\sigma}$  and  $n_{m\sigma}$  create, annihilate and count spin- $\sigma$  particles at lattice site  $m$  and  $\langle mn \rangle$  is a sum denoting nearest neighbour

interactions. [Hint: think about what the favoured (energy lowering) and discouraged (energy raising) terms mean]

We proceed to define these localised orbitals (also called *Wannier orbitals*). First we begin with the eigenstates of the non-interacting Hamiltonian  $\hat{H}^0$  which we denote  $|\psi_{k\sigma}\rangle$  created by operators  $c_{k\sigma}^\dagger$  indexed by a quasi-momentum  $k$ . We then define localised orbitals in terms of these states as

$$c_{n\sigma}^\dagger|\Omega\rangle = |\psi_{n\sigma}\rangle = \frac{1}{\sqrt{N}} \sum_{k[-\pi/a, \pi/a]} e^{ikna} |\psi_{k\sigma}\rangle \quad (4)$$

where  $k = 2\pi m/aN$  with  $-N/2 < m \leq N/2$ . The reverse transform given by,

$$|\psi_{k\sigma}\rangle \equiv \frac{1}{\sqrt{N}} \sum_{n=1}^N e^{-ikna} |\psi_{n\sigma}\rangle \quad (5)$$

- (b) *Argue why for large separations, a Wannier orbital is similar to an isolated atom located around the point  $x = na$ .*

The field operators associated with these orbitals are

$$c_{n\sigma}^\dagger = \int_0^{L=Na} dx \psi_n(x) c_\sigma^\dagger(x), \quad c_\sigma^\dagger(x) = \sum_{n=1}^N \psi_n^*(x) c_{n\sigma}^\dagger \quad (6)$$

where  $\psi_n(x) = \langle x | \psi_{n\sigma} \rangle$ .

- (c) *Show that writing the field operators in terms for the Wannier operators results in*

$$\hat{H} = - \sum_{mn} \sum_{\sigma} t_{mn} c_{m\sigma}^\dagger c_{n\sigma} + \sum_{mnr s} \sum_{\sigma\sigma'} U_{mnr s} c_{m\sigma}^\dagger c_{n\sigma'}^\dagger c_{r\sigma'} c_{s\sigma} \quad (7)$$

where

$$t_{mn} = - \left\langle \psi_m \left| \hat{H}^{(0)} \right| \psi_n \right\rangle = t_{nm}^* \quad (8)$$

are the site hopping matrix elements and

$$U_{mnr s} = \frac{1}{2} \int_0^L dx \int_0^L dx' \psi_m^*(x) \psi_n^*(x') \frac{e^2}{|x-x'|} \psi_r(x') \psi_s(x) \quad (9)$$

are the interaction terms.

So far, all we have done is rewrite the Hamiltonian exactly. Now we can examine some of the terms, identify their meaning and also discard some of them. Consider the interaction term first,

- (d) *For the repeated terms  $U_{mnmn}$  but with  $m \neq n$  explain why these these can be seen as coupling charge densities at different sites. [Hint: the total electron number at site  $m$  is  $\sum_{\sigma} c_{m\sigma}^\dagger c_{m\sigma}$ ]*
- (e) *Repeating the phenomenological arguments you made in part a), show that you indeed recover the effective Hamiltonian from (3).*