

# ICFP M1 - QUANTUM MATTER - TD n°3 - Exercises

## The Hubbard Model

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The Hubbard model describes spin 1/2 fermions hopping on a lattice according to the following tight-binding Hamiltonian:

$$\mathcal{H} = -t \sum_{\sigma} \sum_{\langle i,j \rangle} (c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}) + U \sum_i (\hat{n}_i - 1)^2 - \mu \sum_i (\hat{n}_i - 1) \quad (1)$$

where  $U > 0$  is the repulsive interaction,  $t$  the hopping and  $\mu$  the chemical potential. The sum  $\langle i, j \rangle$  stands for a sum over  $i, j$  nearest neighbor sites on some lattice (in two dimensions this could be a square lattice for instance). As usual for fermions we have:

$$\{c_{i\sigma}, c_{j\sigma'}^{\dagger}\} = \delta_{i,j} \delta_{\sigma\sigma'}. \quad (2)$$

### 1 Particle conservation and $U(1)$ symmetry

1. Let  $\hat{N} = \sum_i \hat{n}_i$  be the total number of particles. Show without any calculation that  $[\hat{N}, \mathcal{H}] = 0$  (as a homework exercise, this can be checked by working through the algebra).
2. Thus  $\hat{N}$  is a conserved quantity. Give the local conservation equation. What is the expression for the corresponding current ?
3. What would be an exemple of a (physical) tight-binding Hamiltonian without particle conservation ?
4. Check that the Hamiltonian is invariant under

$$c_{j\sigma} \rightarrow e^{-i\theta} c_{j\sigma} \quad c_{j\sigma}^{\dagger} \rightarrow e^{i\theta} c_{j\sigma}^{\dagger}. \quad (3)$$

Such a symmetry is called a global  $U(1)$  symmetry. Why is it called a  $U(1)$  symmetry ? And why global ?

5. Let  $U$  be the unitary operator  $U = e^{i\theta \hat{N}}$ . What are  $U c_{j\sigma} U^{\dagger}$  and  $U c_{j\sigma}^{\dagger} U^{\dagger}$  ? Show the equivalence between the global  $U(1)$  symmetry of question 4. and the particle conservation of question 2.

### 2 $SU(2)$ symmetry

6. What are the (global)  $SU(2)$  spin rotation generators in second quantized form ?
7. Is the Hubbard model  $SU(2)$  symmetric ?

Note that the  $U(1)$  and  $SU(2)$  symmetries can be combined into a  $U(2)$  symmetry.

### 3 Particle-hole conjugation

8. For spinless particles, particle-hole conjugation can be defined as a linear, unitary operator  $\Gamma$  such that

$$\Gamma c_i^{\dagger} \Gamma^{\dagger} = c_i \quad (4)$$

If we ignore the  $SU(2)$  symmetry of the Hubbard model, we can define particle-hole conjugation as

$$\Gamma c_{i\sigma}^{\dagger} \Gamma^{\dagger} = c_{i\sigma} \quad (5)$$

Is the  $\mu = 0$  Hubbard model invariant under  $\Gamma$  ?

9. We focus on the Hubbard model on a bipartite lattice, i.e. a lattice which can be partitioned into two sublattices  $A$  and  $B$ , where all the nearest neighbors of  $A$  are members of  $B$ . Show that the sign of  $t$  is unphysical (i.e. one can find a unitary transformation that changes the sign of  $t$ ).

10. It follows from the previous two questions that the Hubbard model (at  $\mu = 0$ ) is in fact particle-hole symmetric on a bipartite lattice. To make this more explicit we consider a slightly modified version of the particle-hole conjugation defined by:

$$\Gamma c_{i\sigma} \Gamma^\dagger = c_{i\sigma}^\dagger \text{ on } A \quad (6)$$

$$\Gamma c_{i\sigma} \Gamma^\dagger = -c_{i\sigma}^\dagger \text{ on } B \quad (7)$$

Check that at  $\mu = 0$  the Hubbard model is indeed invariant under this new  $\Gamma$ . What are the consequences on the spectrum and the eigenstates of  $\mathcal{H}$  ?

11. For spin 1/2 particles the particle-hole conjugation we have defined is not very satisfactory since it does not conserve the spin (it is straightforward to check that  $\Gamma$  changes  $\hat{S} \rightarrow -\hat{S}$ ). It is more natural to define particle-hole conjugation as

$$\Gamma c_{i+} \Gamma^\dagger = c_{i-}^\dagger \quad \Gamma c_{i-} \Gamma^\dagger = -c_{i+}^\dagger \quad \text{on } A \quad (8)$$

$$\Gamma c_{i+} \Gamma^\dagger = -c_{i-}^\dagger \quad \Gamma c_{i-} \Gamma^\dagger = c_{i+}^\dagger \quad \text{on } B \quad (9)$$

To understand why this definition is more natural, compute  $\Gamma \hat{S}_i \Gamma^\dagger$ .

## 4 Weak coupling and strong coupling regimes

12. Some insights can be gained into the Hubbard model by considering the  $t = 0$  limit, in which the different sites decouple. Since the system is now a collection of independent sites, one just needs to solve a single site. What are the eigenstates and energies of a single site ? What is the partition function at inverse temperature  $\beta$  ? What is the density  $\rho = \langle \hat{n}_i \rangle$  ? Plot  $\rho$  versus  $\mu$  for various values of  $\beta$ . What happens at zero temperature ? How is the particle-hole symmetry manifest ?
13. Solve the non-interacting case ( $U = 0$ ) on a one dimensional lattice of  $N$  sites with periodic boundary conditions. What is the dispersion relation ? Is the particle-hole symmetry manifest ?
14. If we want to exactly solve the interacting problem for two sites 1 and 2. What symmetries can one exploit (i.e. what are the good quantum numbers) ?
15. (*Homework*) Determine the spectrum and the eigenstates of the 2-site Hubbard model.

## 5 Strong-coupling regime at half-filling : effective Hamiltonian

We now focus on the Hubbard model at half-filling (we work with a fixed number of particles  $N$ ,  $N$  being the number of sites,  $\mu = 0$ ). In the limit  $U \rightarrow +\infty$ , this model can be (moderately) simplified, notably into the Heisenberg Hamiltonian :

$$\mathcal{H}_H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \quad (10)$$

This effective Hamiltonian can be obtained using perturbation theory at second order around the ground state as we shall see.

16. Find the ground state(s) of the Hubbard model for  $t = 0$ . What is the ground-state degeneracy ?
17. We now consider the regime  $U \gg t$  at half-filling. We want to compute the effective Hamiltonian of the Hubbard model (in the subspace of the previous question). Why do we need to go to second order perturbation theory ? Show that the effective Hamiltonian is the Heisenberg model and specify the effective coupling  $J$ .

**Reminder of perturbation theory:** For  $\mathcal{H} = \mathcal{H}_0 + V$  we perform perturbation theory on  $V$  to second order. We denote  $H_0$  the groundstate of  $\mathcal{H}_0$  of energy  $E_0$ . The effective Hamiltonian can be evaluated on  $H_0$  by

$$\langle \phi' | \mathcal{H}_{\text{eff}} | \phi \rangle = E_0 \langle \phi' | \phi \rangle + \langle \phi' | V | \phi \rangle + \sum_{E_m > E_0} \frac{\langle \phi' | V | m \rangle \langle m | V | \phi \rangle}{E_0 - E_m}. \quad (11)$$