ICFP M1 - QUANTUM MATTER - TD n°3&4 - 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:

$$\mathcal{H} = -t \sum_{\sigma} \sum_{<i,j>} (c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma}) + U \sum_i (\hat{n}_i - 1)^2 - \mu \sum_i (\hat{n}_i - 1) \tag{1}$$

where $U > 0$ is the repulsive interaction, t the hopping and μ the chemical potential. The sum $< i, j >$ 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:

$$\{c_{i\sigma}, c^{\dagger}_{j\sigma'}\} = \delta_{i,j} \delta_{\sigma\sigma'}. \tag{2}$$

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 exercice, 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

$$c_{j\sigma} \to e^{-i\theta} c_{j\sigma} \qquad c^{\dagger}_{j\sigma} \to e^{i\theta} c^{\dagger}_{j\sigma}. \tag{3}$$

   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 $U c^{\dagger}_{j\sigma} U^{\dagger}$? 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 Γ such that

$$\Gamma c^{\dagger}_i \Gamma^{\dagger} = c_i \tag{4}$$

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

$$\Gamma c^{\dagger}_{i\sigma} \Gamma^{\dagger} = c_{i\sigma} \tag{5}$$

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

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 are 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:

$$\Gamma c_{i\sigma}\Gamma^\dagger = c^\dagger_{i\sigma} \text{ on } A \tag{6}$$
$$\Gamma c_{i\sigma}\Gamma^\dagger = -c^\dagger_{i\sigma} \text{ on } B \tag{7}$$

Check that at $\mu = 0$ the Hubbard model is indeed invariant under this new Γ. 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 Γ changes $\hat{S} \to -\hat{S}$). It is more natural to define particle-hole conjugation as

$$\Gamma c_{i+}\Gamma^\dagger = c^\dagger_{i-} \qquad \Gamma c_{i-}\Gamma^\dagger = -c^\dagger_{i+} \qquad \text{on } A \tag{8}$$
$$\Gamma c_{i+}\Gamma^\dagger = -c^\dagger_{i-} \qquad \Gamma c_{i-}\Gamma^\dagger = c^\dagger_{i+} \qquad \text{on } B \tag{9}$$

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 β ? What is the density $\rho = \langle \hat{n}_i \rangle$? Plot ρ versus μ for various values of β. 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 $U \to +\infty$, this model can be (moderately) simplified, notably into the Heisenberg Hamiltonian :

$$\mathcal{H}_\mathrm{H} = J \sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{10}$$

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 effecive Hamiltonian can be evaluated on H_0 by

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