

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

The Hubbard Model

Baptiste Coquinot, Lucile Savary
baptiste.coquinot@ens.fr

2023-2024

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 μ 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

- 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).

All the terms in the Hamiltonian conserve the number of particles (in each term, there are as many destruction as creation operators), so \mathcal{H} commutes with \hat{N} . Physically this simply means that the number of particles (charges for electrons) is conserved.

- Thus \hat{N} is a conserved quantity. Give the local conservation equation. What is the expression for the corresponding current ?

Since \hat{N} is a conserved quantity, we can write a local conservation equation (in the continuum it would be of the form $\partial_t \rho + \nabla \cdot \mathbf{j} = 0$, with $\mathbf{j} = \frac{\hbar}{2im} (\psi^* \nabla \psi - \psi \nabla \psi^*)$). Here, the local density at site i is \hat{n}_i and we define a current operator \hat{J}_{ij} through the link $i \rightarrow j$ (a lattice version of $\nabla \cdot \mathbf{j}$), such that the conservation equation is:

$$\partial_t \hat{n}_i(t) + \sum_{\langle i,j \rangle} \hat{J}_{ij}(t) = 0. \quad (3)$$

Now, we will determine what is \hat{J}_{ij} . In the Heisenberg picture we have:

$$\partial_t \hat{n}_i(t) = i[\mathcal{H}, \hat{n}_i(t)] = -it \sum_{\sigma} \sum_{\langle i,j \rangle} [c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}, c_{i\sigma}^{\dagger} c_{i\sigma}] \quad (4)$$

from which we deduce

$$\hat{J}_{ij} = it \sum_{\sigma} (-c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}). \quad (5)$$

Note that \hat{n}_i evolves with time (it does not commute with \mathcal{H}): the number of particles on site i fluctuates.

- What would be an exemple of a (physical) tight-binding Hamiltonian without particle conservation ?

In superconductivity electrons can form pairs called Cooperons. The nombre of unpaired electrons is not conserved. We have terms like $c_{i+} c_{j-} \Delta_k$ is the Hamiltonian.

- Check that the Hamiltonian is invariant under

$$c_{j\sigma} \rightarrow e^{-i\theta} c_{j\sigma} \quad c_{j\sigma}^{\dagger} \rightarrow e^{i\theta} c_{j\sigma}^{\dagger}. \quad (6)$$

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

By inspection the Hamiltonian is clearly invariant: each term creates as many particles as it annihilates. Such a symmetry is called $U(1)$ (or sometimes S^1) symmetry because the group acting here is the group of complex numbers of modulus one (i.e. phases). More generally $U(n)$ is the group of $n \times n$ unitary matrices (complex matrices such that $U^\dagger U = \text{id}$).

This transformation is allowed since the new creation and annihilation operators have the correct anticommutation relations (we will see in the next question that we are actually dealing with a unitary transformation).

This transformation is called global by opposition to local because θ is not depending of the position i .

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

We check by testing on elementary states that

$$Uc_{j\sigma}U^\dagger = e^{-i\theta}c_{j\sigma} \quad Uc_{j\sigma}^\dagger U^\dagger = e^{i\theta}c_{j\sigma} \quad (7)$$

Global $U(1)$ symmetry means $[e^{i\theta\hat{N}}, \mathcal{H}] = 0$ which is clearly equivalent to $[\hat{N}, \mathcal{H}] = 0$. A conserved quantity corresponds to a Hamiltonian symmetry (Noether theorem) (ex: time translational invariance and energy conservation).

2 $SU(2)$ symmetry

6. What are the (global) $SU(2)$ spin rotation generators in second quantized form?

From the Pauli matrices, we can recover the expression of the spin operators:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (8)$$

$$\hat{S}^x = \sum_i (c_{i+}^\dagger c_{i-} + c_{i-}^\dagger c_{i+}) \quad \hat{S}^y = i \sum_i (c_{i+}^\dagger c_{i-} - c_{i-}^\dagger c_{i+}) \quad \hat{S}^z = i \sum_i (\hat{n}_{i+} - \hat{n}_{i-}) \quad (9)$$

The operators \hat{S}^x and \hat{S}^y can be replaced by

$$\hat{S}^+ = \sum_i c_{i+}^\dagger c_{i-} \quad \hat{S}^- = \sum_i c_{i-}^\dagger c_{i+}. \quad (10)$$

We recall the commutation relations $[\hat{S}_\alpha, \hat{S}_\beta] = i\epsilon_{\alpha\beta\gamma}\hat{S}_\gamma$, from which we can deduce: $[\hat{S}^+, \hat{S}^-] = 2\hat{S}^z$ and $[\hat{S}^z, \hat{S}^\pm] = \pm\hat{S}^\pm$. The rotation of the total spin from an angle ϕ around a vector \mathbf{n} is given by the operator $e^{-i\phi\mathbf{n}\cdot\hat{S}}$.

7. Is the Hubbard model $SU(2)$ symmetric?

Yes, it is. Clearly $[\hat{S}^z, \mathcal{H}] = 0$. The only non-trivial part in showing that $[\hat{S}^+, \mathcal{H}] = 0$ is the kinetic term (indeed $[\hat{S}^+, \hat{n}_i] = 0$). Using $[AB, C] = A\{B, C\} - \{A, C\}B$, one can first derive

$$[\hat{S}^+, c_{i\sigma}^\dagger] = \delta_{\sigma-} c_{i+}^\dagger \quad [\hat{S}^+, c_{i\sigma}] = -\delta_{\sigma-} c_{i+} \quad (11)$$

From this we get $[\hat{S}^+, c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}] = 0$, and we are done.

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

$$\Gamma c_i^\dagger \Gamma^\dagger = c_i \quad (12)$$

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

$$\Gamma c_{i\sigma}^\dagger \Gamma^\dagger = c_{i\sigma} \quad (13)$$

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

Let's compute $\Gamma \mathcal{H} \Gamma^\dagger$. Since

$$\Gamma \hat{n}_{i\sigma} \Gamma^\dagger = 1 - \hat{n}_{i\sigma} \quad (14)$$

the interaction term $U \sum_i (\hat{n}_i - 1)^2$ is indeed invariant.

$$\Gamma (\hat{n}_{i\sigma} - 1)^2 \Gamma^\dagger = (\hat{n}_{i\sigma} - 1)^2 \quad (15)$$

The chemical potential term $-\mu \sum_i (\hat{n}_i - 1)$ changes sign. That has to be expected : if μ is the energy cost of removing an electron, then $-\mu$ is energy cost of removing a hole (i.e adding an electron). So far so good.

But the kinetic term is not invariant :

$$\Gamma (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) \Gamma^\dagger = -(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) \quad (16)$$

To sum things up, the parameters (t, U, μ) of the Hubbard model become $(-t, U, -\mu)$ under the conjugation with Γ . Therefore (on a generic lattice) the Hubbard model is not invariant under particle-hole conjugation (even at $\mu = 0$). But we will see in the following questions that on a bipartite lattice, we do have particle-hole symmetry.

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).

The following local $U(1)$ transformation

$$c_{i\sigma} \rightarrow c_{i\sigma} \text{ on } A \quad (17)$$

$$c_{i\sigma} \rightarrow -c_{i\sigma} \text{ on } B \quad (18)$$

changes the sign of t . This can be achieved with the following unitary transformation

$$U = \prod_{i \in B} (-1)^{\hat{n}_i} \quad (19)$$

Then

$$U (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) U^\dagger = -(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) \quad (20)$$

using that in $\{i, j\}$ exactly one index is on B . This is why on a bipartite lattice we can change the sign of t by acting with U .

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:

$$\Gamma c_{i\sigma} \Gamma^\dagger = c_{i\sigma}^\dagger \text{ on } A \quad (21)$$

$$\Gamma c_{i\sigma} \Gamma^\dagger = -c_{i\sigma}^\dagger \text{ on } B \quad (22)$$

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} ?

We compute

$$\Gamma \mathcal{H} \Gamma^\dagger = -t \sum_{\sigma} \sum_{\langle i, j \rangle} \Gamma (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) \Gamma^\dagger + U \sum_i \Gamma (\hat{n}_i - 1)^2 \Gamma^\dagger - \mu \sum_i \Gamma (\hat{n}_i - 1) \Gamma^\dagger \quad (23)$$

$$= t \sum_{\sigma} \sum_{\langle i, j \rangle} (c_{i\sigma} c_{j\sigma}^\dagger + c_{j\sigma} c_{i\sigma}^\dagger) + U \sum_i (\hat{n}_i - 1)^2 + \mu \sum_i (\hat{n}_i - 1) \quad (24)$$

$$= \mathcal{H} + 2\mu \sum_i \Gamma (\hat{n}_i - 1) \quad (25)$$

We find that under Γ , the chemical potential changes sign. In particular at $\mu = 0$ (half-filling), we have particle-hole symmetry. As the total number of particle \hat{N} commute with the Hamiltonian,

we can solve the problem in fixed number of particles subspaces. Thus, for a lattice of N sites, the subspaces with n particles have the same eigenenergies as the one with $2N - n$ particles and their eigenstates are linked by the particle-hole transformation.

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 $\hat{S} \rightarrow -\hat{S}$). It is more natural to define particle-hole conjugation as

$$\Gamma c_{i+} \Gamma^\dagger = c_{i-}^\dagger \quad \Gamma c_{i-} \Gamma^\dagger = -c_{i+}^\dagger \quad \text{on } A \quad (26)$$

$$\Gamma c_{i+} \Gamma^\dagger = -c_{i-}^\dagger \quad \Gamma c_{i-} \Gamma^\dagger = c_{i+}^\dagger \quad \text{on } B \quad (27)$$

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

We now have

$$\Gamma \hat{n}_{i\sigma} \Gamma^\dagger = 1 - \hat{n}_{i\bar{\sigma}} \quad (28)$$

Again,

$$\Gamma \hat{n}_i \Gamma^\dagger = 2 - \hat{n}_i \quad (29)$$

so that the Hamiltonian remains invariant and

$$\Gamma \hat{S}^z \Gamma^\dagger = \hat{S}^z. \quad (30)$$

Likewise,

$$\Gamma \hat{S}^+ \Gamma^\dagger = \Gamma c_{i+}^\dagger c_{i-} \Gamma^\dagger = c_{i-} c_{i+}^\dagger = \hat{S}^z \quad \Gamma \hat{S}^- \Gamma^\dagger = \hat{S}^- \quad (31)$$

The choice ensures the conservation of \hat{S} . This modified version of the particle-hole conjugation commutes with the $SU(2)$ symmetry. For instance the total spin along the z direction is now preserved under particle-hole conjugation.

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?

For a single site we have the following eigenstates:

- $|0\rangle$ with energy $U + \mu$
- $|+\rangle$ and $|-\rangle$ with energy 0
- $|\pm\rangle$ with energy $U - \mu$

The partition function is

$$Z = \text{Tr}[e^{-\beta\mathcal{H}}] = 2 \left(1 + e^{-\beta U} \text{ch}(\beta\mu) \right) \quad (32)$$

and the density is

$$\rho = \frac{1}{Z} \text{Tr}[\hat{n} e^{-\beta\mathcal{H}}] = \frac{1}{\beta} \partial_\mu \ln(Z) + 1 = \frac{2e^{-\beta(U-\mu)} + 2}{2 + e^{-\beta(U-\mu)} + e^{-\beta(U+\mu)}}. \quad (33)$$

At zero temperature the mean occupation is discontinuous :

$$\rho = \begin{cases} 0 & \text{for } \mu < -U \\ 1 & \text{for } -U < \mu < U \\ 0 & \text{for } U < \mu \end{cases} \quad (34)$$

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?

We use the translation invariance by going to the Fourier space. We define

$$d_{k\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_j c_{j\sigma}^\dagger e^{ikj} \quad (35)$$

for $k = \frac{2\pi}{N}m$ with $m = 0, \dots, N-1$. They fulfil the usual anti-commutation relation. The usual resolution gives

$$\mathcal{H} = \sum_{k,\sigma} (\epsilon_k - \mu) \hat{n}_{k,\sigma} \quad (36)$$

where $\epsilon_k = -2t \cos(k)$. The particle-hole symmetry is there (assuming that $\mu = 0$ and that N is even!), but is not particularly easy to see. For instance one can check that the empty and full occupied system have the same energy. Using the two sublattices, Γ transforms $\Gamma d_{k,\sigma}^\dagger \Gamma^\dagger = d_{\pi-k,\sigma}^\dagger$.

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) ?

The symmetries that can be used are:

- the total particle number \hat{N}
- the total spin \hat{S} ,
- the exchange symmetry between the two sites \hat{P}
- the particle hole symmetry Γ .

But to be useful, these symmetries must be limited to a set of commuting symmetries. For example, Γ et \hat{N} do not commute, nor the different components of the total spin operator \hat{S} each with the other: they are not compatible and cannot be simultaneously diagonalized. Γ , \hat{S}^x and \hat{S}^y are thus eliminated. Then, we can add the squared spin operator \hat{S}^2 , that commutes with each of the spin components and whose eigenvalues are $S(S+1)$ with S the total spin of the state.

We denote the corresponding quantum numbers by (N, S^z, S, P) . The Hubbard Hamiltonian is block diagonal with respect to these quantum numbers.

15. (*Homework*) Determine the spectrum and the eigenstates of the 2-site Hubbard model.

Contact me to discuss the solution.

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 :

$$\mathcal{H}_H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \quad (37)$$

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 ?

In the ground state, there is exactly one particle per site. It leads to a degeneracy of 2^N with N the number of sites. We have for each site the possibility to place a + or - spin particle.

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 .

We use a perturbation theory with

$$\mathcal{H}_0 = U \sum_i (\hat{n}_i - 1)^2 \quad V = -t \sum_{\sigma} \sum_{\langle i,j \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) \quad (38)$$

The ground state of \mathcal{H}_0 has been determined in the previous question and have energy $E_0 = 0$. The excited states are all the other ones, namely those with a least an empty site or a doubly occupied one. When acting with V on a ground state, we get terms like $c_{i\sigma}^\dagger c_{j\sigma}$ that takes an electron from site j and move it to site i . Starting from a ground state, we end up with a (linear combination of) state with $\hat{n}_i = 2$ and $\hat{n}_j = 0$, i.e. a state $|m\rangle$ with energy (under \mathcal{H}_0) $E_m = U$. Therefore, the first order perturbation theory vanishes, and we need to go to second order where two electrons are exchanged. At second order we get

$$\langle \sigma'_1 \dots \sigma'_N | \mathcal{H}_{\text{eff}} | \sigma_1 \dots \sigma_N \rangle = - \sum_{|m\rangle} \frac{\langle \sigma'_1 \dots \sigma'_N | V | m \rangle \langle m | V | \sigma_1 \dots \sigma_N \rangle}{E_m} \quad (39)$$

where $|m\rangle$ are excitations around the eigenstate. The V bring sums over $\langle i, j \rangle$ and $\langle i', j' \rangle$. The only nonvanishing terms are for $i = i'$ and $j = j'$ (or the symmetrical) and $|m\rangle = c_{i\sigma}^\dagger c_{j\sigma} | \sigma_1 \dots \sigma_N \rangle$ or $|m\rangle = c_{j\sigma}^\dagger c_{i\sigma} | \sigma_1 \dots \sigma_N \rangle$. Both have the energy $E_m = 2U$. Therefore,

$$\langle \sigma'_1 \dots \sigma'_N | \mathcal{H}_{\text{eff}} | \sigma_1 \dots \sigma_N \rangle = - \frac{t^2}{2U} \sum_{\langle i,j \rangle, \sigma\sigma'} \langle \sigma'_1 \dots \sigma'_N | c_{j\sigma'}^\dagger c_{i\sigma'} c_{j\sigma}^\dagger c_{i\sigma} + c_{i\sigma'}^\dagger c_{j\sigma'} c_{i\sigma}^\dagger c_{j\sigma} | \sigma_1 \dots \sigma_N \rangle \quad (40)$$

Therefore, the effective Hamiltonian is

$$\mathcal{H}_{\text{eff}} = - \frac{t^2}{2U} \sum_{\langle i,j \rangle, \sigma\sigma'} (c_{j\sigma'}^\dagger c_{i\sigma'} c_{j\sigma}^\dagger c_{i\sigma} + c_{i\sigma'}^\dagger c_{j\sigma'} c_{i\sigma}^\dagger c_{j\sigma}) = - \frac{t^2}{2U} \sum_{\langle i,j \rangle, \sigma\sigma'} (-2c_{i\sigma}^\dagger c_{i\sigma'} c_{j\sigma'}^\dagger c_{j\sigma} + \delta_{\sigma\sigma'} (\hat{n}_{i\sigma} + \hat{n}_{j\sigma})) \quad (41)$$

Using that $\hat{n}_i = \hat{n}_j = 1$ we find

$$\mathcal{H}_{\text{eff}} = \frac{t^2}{U} \sum_{\langle i,j \rangle, \sigma\sigma'} \left(c_{i\sigma}^\dagger c_{i\sigma'} c_{j\sigma'}^\dagger c_{j\sigma} - \frac{1}{4} \right) \quad (42)$$

We can separate the sum over σ, σ' into terms where $\sigma = \sigma'$ and terms where $\sigma = -\sigma'$ to recognise

$$\sum_{\sigma\sigma'} c_{i\sigma}^\dagger c_{i\sigma'} c_{j\sigma'}^\dagger c_{j\sigma} = \sum_{\sigma} \hat{n}_{i\sigma} \hat{n}_{j\sigma} + \hat{S}_i^+ \hat{S}_i^- + \hat{S}_i^- \hat{S}_i^+ = \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j. \quad (43)$$

Up to a constant to recover the Heisenberg Hamiltonian with $J = 2t^2/U$. Since $U > 0$, we expect ferromagnetic order.

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

$$\langle \phi' | \mathcal{H}_{\text{eff}} | \phi \rangle = E_0 \langle \phi' | \phi \rangle + \langle \phi' | V | \phi \rangle + \sum_{E_m > E_0} \frac{\langle \phi' | V | m \rangle \langle m | V | \phi \rangle}{E_0 - E_m}. \quad (44)$$