Tutorials of Theoretical Condensed Matter 2019-2020

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The Hubbard model

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

$$\hat{H}_{\mathrm{Hub}} = -t \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_{\langle i,j \rangle} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i (\hat{n}_i - 1)^2 - \mu \sum_i (\hat{n}_i - 1), \qquad \hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} \tag{1}$$

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:

$$\begin{aligned} \left\{ c_{i\sigma}, c^\dagger_{j\sigma'} \right\} &= \delta_{i,j}\, \delta_{\sigma,\sigma'} \\ \left\{ c_{i\sigma}, c_{j\sigma'} \right\} &= 0 \\ \left\{ c^\dagger_{i\sigma}, c^\dagger_{j\sigma'} \right\} &= 0 \end{aligned} \tag{2}$$

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 $[\hat{N}, \hat{H}_{\mathrm{Hub}}] = 0$ (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

$$c_{j\sigma} \to e^{-i\theta} c_{j\sigma}, \qquad c^\dagger_{j\sigma} \to e^{i\theta} c^\dagger_{j\sigma}$$

   Is such a transformation allowed ? 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 2. and the particle conservation of question 1.

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

$$c^\dagger_{j\sigma} \to \sum_{\sigma'} V_{\sigma\sigma'} c^\dagger_{j\sigma'}, \qquad V \in U(2)$$

   Indeed a generic matrix V in U(2) can be decomposed as

$$V = e^{i\theta} W, \qquad W \in SU(2)$$

   and is therefore the product of $U(1)$ and a SU(2) unitary transformation.

3 Particle-hole conjugation

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

$$\Gamma c^\dagger_i \Gamma^\dagger = c_i$$

   (homework : does such an operator exist ? is it unique ? What is $\Gamma|0\rangle$?)

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

$$\Gamma c^\dagger_{i\sigma} \Gamma^\dagger = c_{i\sigma}$$

   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:

$$\begin{aligned} \Gamma c^\dagger_{i\sigma} \Gamma^\dagger &= c_{i\sigma} \quad \text{on the } A \text{ sublattice,} \\ \Gamma c^\dagger_{i\sigma} \Gamma^\dagger &= -c_{i\sigma} \quad \text{on the } B \text{ sublattice.} \end{aligned}$$

   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 $\hat{H}_{\text{Hub}}$?

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

$$\Gamma c^\dagger_{i\uparrow} \Gamma^\dagger = c_{i\downarrow}, \qquad \Gamma c^\dagger_{i\downarrow} \Gamma^\dagger = -c_{i\uparrow}$$

   (homework : does such an operator exist ? is it unique ?). To understand why this definition is more natural, compute $\Gamma \hat{S}_i \Gamma^\dagger$.

   Putting all this together, we are led to define the following particle-hole conjugation :

$$\begin{aligned} \tilde{\Gamma} c^\dagger_{i\uparrow} \tilde{\Gamma}^\dagger = c_{i\downarrow} \quad \text{and} \quad \tilde{\Gamma} c^\dagger_{i\downarrow} \tilde{\Gamma}^\dagger = -c_{i\uparrow} \quad \text{on the } A \text{ sublattice,} \\ \tilde{\Gamma} c^\dagger_{i\uparrow} \tilde{\Gamma}^\dagger = -c_{i\downarrow} \quad \text{and} \quad \tilde{\Gamma} c^\dagger_{i\downarrow} \tilde{\Gamma}^\dagger = c_{i\uparrow} \quad \text{on the } B \text{ sublattice.} \end{aligned}$$

   We now have

$$\tilde{\Gamma} \hat{H}_{\text{Hub}}(\mu) \tilde{\Gamma}^\dagger = \hat{H}_{\text{Hub}}(-\mu), \qquad \tilde{\Gamma} \hat{S}^\mu \tilde{\Gamma}^\dagger = \hat{S}^\mu, \qquad \tilde{\Gamma} \hat{N} \tilde{\Gamma} = 2N - \hat{N}. \tag{3}$$

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 ? As a homework exercice, what would be the dispersion relation on a two-dimensional $N \times N$ square lattice ?

5 Exact solution for 2 sites

14. We choose 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. Determine the spectrum and the eigenstates.

6 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).

$$H_{\text{Hub}} = -t \sum_{\langle ij \rangle, \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i (n_i - 1)^2,$$

In the limit $U \to \infty$, this model can be (moderately) simplified, notably into the Heisenberg Hamiltonian :

$$H_{\text{Heis}} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j,$$

This effective Hamiltonian can be obtained using perturbation theory (see Appendix).

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

$$H_{\text{Heis}} = \frac{2t^2}{U} \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j,$$

A Perturbation theory

We recall here some results of degenerate perturbation theory for an Hamiltonian $\hat{H} = \hat{H}_0 + \lambda \hat{V}$ for $\lambda \to 0$. We denote by $\mathcal{H}_0$ the ground state subspace, with energy E_0. To second order in perturbation theory, the effective Hamiltonian in $\mathcal{H}_0$ is

$$\hat{H}_{\text{eff}} = E_0 P + \lambda \hat{P} \hat{V} \hat{P} + \lambda^2 P V Q (E_0 - Q H_0 Q)^{-1} Q V P$$

where P is the projector on $\mathcal{H}_0$ and $Q = 1 - P$. This can be reformulated as follow. For two states $|\phi\rangle$, $|\phi'\rangle$ in $\mathcal{H}_0$, we have

$$\langle \phi' | \hat{H}_{\text{eff}} | \phi \rangle = E_0 \langle \phi' | \phi \rangle + \lambda \langle \phi' | \hat{V} | \phi \rangle + \lambda^2 \sum_{|m\rangle \notin \mathcal{H}_0} \frac{\langle \phi' | V | m \rangle \langle m | V | \phi \rangle}{E_0 - E_m}$$

where the sum runs over all eigenvectors $|m\rangle$ (of H_0) not in $\mathcal{H}_0$.

Note : it is a good exercice to derive this formula.