Computational Quantum Physics
Exercise 7

FS 16
Prof. S. Huber

Problem 7.1 The Tight-Binding Model

In this exercise we will solve the tight-binding model

$$H = \sum_{\langle i,j\rangle,\sigma} \left(t_{ij} c^\dagger_{i,\sigma} c_{j,\sigma} + h.c. \right) \tag{1}$$

on the square lattice analytically. We will assume uniform hopping amplitudes $t_{ij} = -t$.

Bring the Hamiltonian into the diagonal form

$$H = \sum_{\mathbf{k},\sigma} \epsilon(\mathbf{k}) n_{\mathbf{k},\sigma} \tag{2}$$

and identify the dispersion relation $\epsilon(\mathbf{k})$.

Hint: Assuming the lattice has $N = L \times L$ sites with spacing a and periodic boundary conditions, you can replace the field operators by their Fourier transforms using

$$c_{i,\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r_i}} c_{\mathbf{k},\sigma}, \tag{3}$$

where the lattice momenta run over N points of the Brillouin zone

$$\mathbf{k} = \frac{2\pi}{aL}(n_x, n_y), \qquad n_{x,y} = \{0, \ldots, L-1\}. \tag{4}$$

Problem 7.2 Exact Diagonalization of 2-site Lattice Hamiltonians

The most accurate method for solving a quantum many-body problem is exact diagonalization of the Hamiltonian matrix. In order to make the most out of the computational resources available, it is very helpful to make use of all available tools for simplifying the problem.

In this exercise we will have a closer look at the steps involved in making use of symmetries of the Hamiltonian. Specifically, we will construct the Hamiltonian matrix for a few different models on a two-site lattice and break it down into blocks corresponding to different symmetry sectors.

For each of the models described below follow these steps:

- Choose a basis adequate for the degrees of freedom involved in the problem.
- Construct the Hamitonian matrix H using the above basis.
- Identify the different symmetries of the model and organize your basis so that basis elements corresponding to the same symmetry sector are grouped up together.[1]
- Diagonalize the blocks corresponding to each individual symmetry sector.

[1] Notice that at this point a full construction of the Hamiltonian matrix should reveal the block diagonal structure corresponding to the different symmetry sectors.

Models

1. **Spin-1/2 Heisenberg model**[2]

$$H = J\vec{S}_1 \cdot \vec{S}_2 \tag{5}$$

for $J = \pm 1$. Here, the spin operators can be written in terms of the Pauli matrices $\vec{S} = \frac{\hbar}{2}(\sigma_x, \sigma_y, \sigma_z)^T$.

2. **Spin-1 Heisenberg model**[3] Same Hamiltonian as above, but this time the $\vec{S}_i$ are Spin-1 operators. *Hint:* Express $S_{x,y}$ in terms of the ladder operators $S_\pm$ as demonstrated in the lecture notes.

3. **Bose-Hubbard model**[4]

$$H = -t\left(b_1^\dagger b_2 + b_2^\dagger b_1\right) + \frac{U}{2}\sum_{i=1}^{2} n_i\left(n_i - 1\right) \tag{6}$$

Here the two sites can be occupied by spinless bosons ($b_i^{(\dagger)}$: bosonic annihilation (creation) operators). As each site could hold an arbitrary number of bosons, you have to limit the total number of particles, e.g. to $N_{max} = 4$. Fix $t = 1$ and diagonalize the system for $U = -1, 1, 4$. For which cases does the particle number cut-off seem reasonable?

4. **(Fermi-) Hubbard model**[5]

$$H = -t\sum_{\sigma=\uparrow,\downarrow}\left(c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}\right) + U\sum_{i=1}^{2} n_{i\uparrow}n_{i\downarrow}. \tag{7}$$

Here the local degrees of freedom correspond to fermions carrying a spin-1/2.

5. $t - J$ **model**[6]

$$H = -t\sum_{\sigma=\uparrow,\downarrow}\Big(\left(1 - n_{1,-\sigma}\right)c_{1\sigma}^\dagger c_{2\sigma}\left(1 - n_{2,-\sigma}\right) + h.c.\Big) + J\left(\mathbf{S}_1 \cdot \mathbf{S}_2 - \frac{n_1 n_2}{4}\right) \tag{8}$$

Here the local degrees of freedom correspond to fermions carrying a spin-1/2 with the exception that double occupancies are forbidden.

[2] See discussion in 8.5.3 of the lecture notes

[3] See discussion in 8.5.3 of the lecture notes

[4] This is the equivalent of the Hubbard model discussed in 8.5.2 of the lecture notes in the case of spinless bosons

[5] See discussion in 8.5.2 of the lecture notes

[6] See discussion in 8.5.4 of the lecture notes