Computational Quantum Physics Exercise 4

FS 12
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Problem 4.1 Tight binding model

In this exercise you 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 simple square lattice analytically. You can assume uniform hopping amplitudes $t_{ij} = t$. Assuming the lattice has $N = L \times L$ sites with spacing a and periodic boundary conditions, you replace the field operators by their Fourier transform

$$c_{i,\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x_i}} c_{\mathbf{k},\sigma}, \tag{2}$$

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

$$\mathbf{k} = \frac{2\pi}{aL}(n_x, n_y), \qquad n_{x,y} = \{0, \ldots, L-1\}. \tag{3}$$

Bring the Hamiltonian into the diagonal form

$$H = \sum_{\mathbf{k},\sigma} \epsilon(\mathbf{k}) n_{\mathbf{k},\sigma} \tag{4}$$

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

Problem 4.2 Exact diagonalization of lattice Hamiltonians

The most accurate method for solving a quantum many-body problem is exact diagonalization of the Hamiltonian matrix. In this exercise we will have a close look at the first two steps of this task: For different models on a two-site lattice we will construct the Hamiltonian matrix and break it down into blocks corresponding to different symmetry sectors.

For each of the models described below

- write down the full Hamiltonian matrix H in a sensible basis,
- partition the basis states into sectors such that H matrix elements between states from different sectors vanish,
- diagonalize the block of H belonging to each sector.

What are the physical symmetries that allow you to split the Hamiltonians into blocks?

Models

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

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

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** 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 script.

3. **Bose-Hubbard model**

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

Now 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 $U = -1, 1, 2$. Which cases does the particle number cut-off seem reasonable for?

4. **(Fermi-) Hubbard model** This is the regular Hubbard model with fermions carrying a spin-1/2 as described in in chapter 6 of the lecture script.

5. $t - J$ **model** This Hamiltonian is also introduced in the script.