Computational Quantum Physics Exercise 4

PHYS-463
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Problem 4.1 The Tight-Binding Model

In this exercise we analytically solve the tight-binding model

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

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

Bring the Hamiltonian into the diagonal form

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

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

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

where the lattice momenta $\mathbf{k}$ 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 4.2 Exact Diagonalization of the Bose-Hubbard model

We consider the Bose-Hubbard model, given by the hamiltonian

$$\hat{H} = -t \sum_{\langle i,j\rangle} \left(\hat{b}^{\dagger}_i \hat{b}_j + \hat{b}^{\dagger}_j \hat{b}_i \right) + \frac{U}{2} \sum_i \hat{n}_i \left(\hat{n}_i - 1 \right) - \mu \sum_i \hat{n}_i$$

Here the 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 $< d = 5$.

- Choose an adequate basis for the degrees of freedom involved. Fix $t = 1$ and $\mu = 0$. For $U = -1, 1, 4$ construct the above Hamiltonian in that basis and diagonalize it. For which cases does the particle number cut-off seem reasonable?

  Hint: Follow the approach in Section 5.4.1 of the lecture notes.

- We know that $[\hat{H}, \hat{N}] = 0$, therefore all eigenstates $|\psi_i\rangle$ of $\hat{H}$ have a fixed number of particles. Compute the number of particles of each eigenstate $\langle\psi_i|\hat{N}|\psi_i\rangle$.

- Since $[\hat{H}, \hat{N}] = 0$, this is a symmetry of the system. Use this fact to find the ground state for a fixed number of particles using the power method (by changing the initial guess).

Problem 4.3 Exact diagonalization of the t-V model

Implement exact diagonalization for the 1-dimensional t-V model of length L with a potential V.

$$\hat{H} = t \sum_{\langle i,j \rangle} \left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \right) + V \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j$$

For the numerical implementation, you can fix $t = 1$ and $V = 1$.

- Use the Jordan-Wigner transform as described in section 5.4.2 of the lecture notes to write the annihilation operator $\hat{c}_i$ in terms of kronecker products of spin operators. Implement a function which constructs the corresponding sparse matrix and use it to construct the whole hamiltonian.
- Use a sparse eigenvalue solver to find the ground state energy for the periodic and non-periodic case for some system sizes (2,4,6,8,10,12, ...).

  For the ground state at open boundary conditions, you can find some reference results below:

L	Energy per site
2	-0.5000
3	-0.4714
4	-0.5000
5	-0.5177
⋮	⋮

- Use again $[\hat{H}, \hat{N}] = 0$ to find the ground state for a fixed number of particles using the power method with an appropriate initial guess.
- (optional): Block-diagonalize the Hamiltonian matrix and make use of the resulting structure to speed up the ED calculation.

Problem 4.4 Exact diagonalization of the Fermi-Hubbard model

Study the Fermi-Hubbard model given by the Hamiltonian

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \left(\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}.$$

with exact diagonalization. Here the local degrees of freedom correspond to fermions carrying spin-1/2.
Hint: Use the procedure described in section 5.4.2 of the lecture notes to map it to a problem of spinless fermions and use a Jordan-Wigner transform like in Problem 4.3.