Exercise for Computational Materials Sciences

Exercise 4, December 6th, 2024. Discussion on Decmeber 17th, 2024

1) Hubbard atom

Consider the Hubbard model for a system of just one site:

$$H = -\mu \sum_{\sigma} c_{\sigma}^{\dagger} c_{\sigma} + U n_{\downarrow} n_{\uparrow}, \tag{1}$$

$\sigma = \downarrow, \uparrow$ being the spin, and $n_{\sigma} = c_{\sigma}^{\dagger} c_{\sigma}$ being the particle number operator of a given spin.

a) Show that $|0\rangle$, $|\uparrow\rangle = c_{\uparrow}^{\dagger}|0\rangle$, $|\downarrow\rangle = c_{\downarrow}^{\dagger}|0\rangle$, and $|\uparrow\downarrow\rangle = c_{\uparrow}^{\dagger} c_{\downarrow}^{\dagger}|0\rangle$ are eigenstates of H. Calculate the partition function $Z = \mathrm{Tr} e^{-\beta H}$ and the average occupation $\langle n_{\downarrow} + n_{\uparrow} \rangle$ as a function of the chemical potential μ and the inverse temperature β.

b) Plot N as a function of μ for $U = 4$ and $\beta = 1/2$. To what chemical potential does the half-filling ($N = 1$) correspond?

c) Calculate and plot the local magnetic moment $\langle m^2 \rangle = \langle (n_{\uparrow} - n_{\downarrow})^2 \rangle$ at half-filling as a function of temperature $T = 1/\beta$. Give a qualitative explanation of why for high temperatures ($T \gg U$) $\langle m^2 \rangle = \frac{1}{2}$ and for low temperatures ($T \ll U$) $\langle m^2 \rangle = 1$.

In the typical research context, the Hamiltonian will be too complicated to diagonalize by hand. Computers can help by finding *numerical solutions* in these cases. Write a python script that calculates the average occupation and the local magnetic moment of the Hubbard atom for a given value of U, μ, and β. Then:

d) Plot the numerically computed average occupation vs. the chemical potential in accordance with **b)**.

e) Plot the numerically computed local magnetic moment vs. the temperature in accordance with **c)**.

Do your numerical results agree with your analytical expressions?

2) The Hubbard dimer

Consider a two-site Hubbard model with the hopping matrix elements $t_{12} = t_{21} = t$ where $t > 0$ and the local Coulomb interaction parametrized by U,

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

The two-site Hubbard model, the Hubbard dimer, can be considered as model system for the correlation effects present in a chemical bond.

a) Diagonalize the Hamiltonian and obtain the analytical expression for the eigen-values. **Hint:** Use the fact that Hubbard Hamiltonian is number and spin conserving and write the Hamiltonian in block-diagonal form.

b) Sketch the behavior of filling i.e. $N(\mu) = \sum_{i\sigma} \langle n_{i\sigma} \rangle$ as a function of chemical potential μ. The thermal average of operator $\hat{O}$ is defined as,

$$\langle \hat{O} \rangle = \frac{\mathrm{Tr}\left(\hat{O} e^{-\beta \hat{H}}\right)}{\mathrm{Tr}\left(e^{-\beta \hat{H}}\right)} \tag{3}$$

For a given interaction parameter U and inverse temperature β, which values of chemical potential leads to half-filling i.e. $N = 2.0$?

c) At half-filling, evaluate the on-site magnetization $m_i = \langle (n_{i\uparrow} - n_{i\downarrow})^2 \rangle$ as a function of $\frac{U}{t}$ for low temperatures.

d) Obtain the ground-state in the mean-field limit ($n_{i\sigma} \to \langle n_{i\sigma} \rangle$) and compare it with the exact results.

d) Support your analytical results with numerical diagonalization.