Exercise for Theoretical Condensed Matter Physics

Exercise 2, April, 11th 2024. Discussion on April, 22nd 2024

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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 $Z = e^{-\beta H}$ 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?

Tips and tricks:

- You might find the following commonly-used scientific python packages useful: numpy (numpy array objects represent matrices and vectors), scipy (library of mathematical algorithms including linear algebra routines), and matplotlib (plotting functionality).
- If you are new to python programming or need a refresher, take a quick look through the python tutorials section from TRIQS, especially the first three subsections under *Basics*.
- It is good practice to maintain separate *environments* for different research projects. For this course, please use the conda package manager. The easiest way to start with conda is to use the free Anaconda distribution.
- iPython notebooks are extremely useful for developing and debugging code. Please use Jupyter notebooks that come bundled with the Anaconda distribution.

A preview of the next exercise sheet:

In condensed matter research, we go one step further. Rather than simply using the standard python libraries (numpy, scipy, etc), we write our programs over another layer of condensed matter specific libraries which have efficient representations and implementations of the most commonly used objects and algorithms in condensed matter physics.

In the next exercise sheet, you will use TRIQS (Toolbox for Research on Interacting Quantum Systems) to solve the Hubbard atom as well as a more complex problem. You may already install TRIQS (please use the Anaconda package manager) and familiarize yourself with some of its functionality, as described on this page.