Exercise for Theoretical Condensed Matter Physics

Exercise 3, April, 19th 2024. Discussion on April, 29th 2024

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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,

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

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,

$$\langle \hat{O} \rangle = \frac{\text{Tr}\left(\hat{O} e^{-\beta \hat{H}} \right)}{\text{Tr}\left(e^{-\beta \hat{H}} \right)} \tag{2}$$

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.

e) Support your conclusions with numerical results using the atom_diag module from TRIQS. The companion Jupyter notebook *Ex_03_companion.ipynb* will guide you through the task. When in doubt, refer to the atom_diag or TRIQS documentation. Good starting points are here and here.