Quantum phase transitions

Exercise Sheet 7

In this exercise we consider the Bose-Hubbard model on a translationally invariant lattice with coordination number z:

$$\hat{\mathcal{H}} = -t \sum_{\langle ij \rangle} \hat{b}_i^\dagger \hat{b}_j + \text{h.c.} + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) - \mu \sum_i \hat{n}_i. \tag{1}$$

We will try to locate the Mott-insulator (MI) to super-fluid (SF) phase transition using a mean-field variational ansatz known as the Gutzwiller wavefunction:

$$|\Psi\rangle \equiv |\Phi\rangle \otimes |\Phi\rangle \otimes \cdots \otimes |\Phi\rangle, \quad |\Phi\rangle \equiv \sum_{n=0}^{N} a_n |n\rangle, \tag{2}$$

where $|n\rangle$ is the normalized local state with n bosons, and a_n are variational parameters that we can take to be real. The wavefunction $|\Psi\rangle$ is a general translationally invariant product state.

Contrary to the Hamiltonian (1), the ansatz $|\Psi\rangle$ does not conserve the local particle number for general a_n, so there may be non-zero fluctuations $v \equiv \langle \hat{n}^2 \rangle - \langle \hat{n} \rangle^2$.

We take the limit where system size and the number of particles go to infinity while the particle density $\bar{n}$ remains constant. In practice, we maintain a cutoff N in the local occupation so as to have a finite number of variational parameters, which is perfectly valid if N^2 is much greater than the particle number fluctuations v.

In the classical limit $t = 0$, the system is in a Mott insulator state characterized by integer $\bar{n} = 1, 2, \ldots$ for $\bar{n} - 1 < \mu/U < \bar{n}$. We tune the chemical potential μ to the middle of these intervals where the MI phases are supposedly the most stable:

$$\mu = U(\bar{n} - 1/2). \tag{3}$$

By setting $U = 1$ as our energy scale and tuning t, we will probe the MI-SF transition.

1. What should a_n be when we are deep inside an MI phase? What is the resulting v?

2. The local particle number $\langle \hat{n} \rangle$ of our wavefunction should be $\bar{n}$ inside an MI phase.[1] What is the resulting condition on the a_n?

3. In the $U \to 0$ limit, the ground state is a Bose-Einstein condensate of quasiparticles of momentum $\vec{k} = \vec{0}$. Calculate the local fluctuations v in the ground state on a finite system, then take the limit of large system size to verify that the local number of particles is similar to a Poisson random variable, justifying the approximation of the SF ground state by

$$a_n^2 = \frac{m^n e^{-m}}{n!}. \tag{4}$$

Determine m given the constraints above.

[1] This condition should also be valid in the SF phase along line (3) when we are close to the transition since the lines of integer occupation in the SF phase seem to meet the MI phases at the tip of the lobes.

4. We will determine the a_l numerically by minimizing the energy $\langle \hat{\mathcal{H}} \rangle$ of the Gutzwiller wavefunction while requiring normalization of the wavefunction and $\langle \hat{n} \rangle = \bar{n}$, which suggests the use of the Lagrange multipliers method. We define the Lagrangian

$$\mathcal{L}(\vec{a}, \lambda_1, \lambda_2) \equiv \langle \hat{\mathcal{H}} \rangle (\vec{a}) - \lambda_1 g_1(\vec{a}) - \lambda_2 g_2(\vec{a}), \tag{5}$$

where $(\vec{a})_l \equiv a_l$. Calculate the gradient $\vec{\nabla}_{(\vec{a},\lambda_1,\lambda_2)} \mathcal{L}$ and write a script that will compute it.

Suggestion: Complete the script ex.py provided.

5. Using a numerical root finder, complete your script to solve $\vec{\nabla} \mathcal{L} = \vec{0}$ and determine a_l.

Note: A good initial guess for the a_l is essential to obtain the right minimum of $\mathcal{L}$. In the neighborhood of the critical point, using a Poisson distribution as the starting point should work well on both sides of the transition, at least when using the solver specified in ex.py.

6. What quantities are appropriate to probe the phase transition? Find an "order parameter" which is non-zero only in one of the phases. You can use first or second (numerical) derivatives of the energy or the order parameter to identify the critical zt_c, for different $\bar{n}$.

7. As a reference for $\bar{n} = 1$, more accurate numerical and analytical methods have found $t_c \approx 0.29$ for a 1D chain, $t_c \approx 0.061$ for a square lattice, and $t_c \approx 0.034$ for a cubic lattice. Compare with your findings.