2008 Oxford summer school on cold atoms

Problem sheet, D Jaksch

1. **The Gutzwiller approximation**

Ultracold bosonic atoms in a 1D optical lattice are described by the Bose-Hubbard Hamiltonian

$$H = -J \sum_m \left(a_m^\dagger a_{m+1} + \text{h.c.} \right) + \frac{U}{2} \sum_m a_m^\dagger a_m^\dagger a_m a_m - \mu N \ .$$

Here J is the hopping matrix element, U the onsite atom-atom interaction, μ the chemical potential and N the particle number operator. The bosonic operator a_m destroys a particle in site m. In the Gutzwiller approximation the state of the atoms in the lattice is written as

$$|G\rangle = \prod_{m=1}^{M} \left(\sum_n f_n^{(m)} |n\rangle_m \right) ,$$

where $|n\rangle_m$ is a Fock state of n atoms in site m. We investigate how this state describes the superfluid and Mott insulator regions, and the transition between them.

(i) Show that $|G\rangle$ is a matrix product state.

(ii) Calculate $f_n^{(m)}$ so that $|G\rangle$ becomes the Mott insulating ground state of H for $J = 0$. How does the lattice site occupation n change with μ. Calculate the particle number fluctuations in lattice site m.

(iii) We introduce a small perturbation to the $n = 1$ Mott insulator

$$|G_\epsilon\rangle = \mathcal{N} \prod_m \left(\sqrt{\epsilon}\, |0\rangle_m + |1\rangle_m + \sqrt{\epsilon}\, |2\rangle_m \right) \ .$$

Calculate the normalization factor $\mathcal{N}$ and show that this state preserves the average particle number when varying ϵ. By working out the energy expectation value $\langle G_\epsilon | H | G_\epsilon \rangle$ conclude that the Mott insulator becomes unstable at a critical value of

$$\left(\frac{U}{2J} \right)_{crit} \approx 5.8.$$

(iv) In the limit $J \gg U$ the ansatz

$$|G\rangle \propto e^{\sum_m \phi_m a_m^\dagger} |\text{vac}\rangle \ ,$$

is a good approximation. Calculate the corresponding values of $f_n^{(m)}$. Assume the parameters ϕ_m to be time dependent and find their evolution equation from a variational calculation, i.e. minimizing $\langle G | \mathrm{i}\partial_t - H | G \rangle$. Show that this recovers a discretized form of the Gross-Pitaevskii equation. By going to the continuum limit identify the macroscopic wave function, effective mass and interaction coefficient g of the lattice system. Calculate the particle number fluctuations in lattice site m in this limit.

(v) Discuss the importance of the possibility of violating particle number conservation in the state $|G\rangle$ for describing the superfluid state. There are no correlations between the different lattice sites in this approximation. Is this consistent with the description of a BEC using a macroscopic wave function?

2. **Matrix product states**

We consider a one dimensional optical lattice of M sites which each can either be empty or filled with one particle. We denote these two quantum states per site as $\{|\uparrow\rangle, |\downarrow\rangle\}$. Pauli matrices are denoted as σ's in the standard way in this problem.

(i) Write the fully polarized states $|\Uparrow\rangle = |\uparrow\uparrow\cdots\uparrow\rangle$ and $|\Downarrow\rangle = |\downarrow\downarrow\cdots\downarrow\rangle$ as matrix product states with matrices A and B, respectively.

(ii) Use the above result to show that the superposition $|\Uparrow\rangle + |\Downarrow\rangle$ can be written as a matrix product state with matrices $C = A \oplus B$ for periodic boundary conditions (PBC). Show that the matrix product is canonical for PBC and for suitably chosen boundary states $|\Phi_0\rangle$ and $|\Phi_M\rangle$ also in the case of open boundary conditions (OBC).

(iii) Extract the Schmidt decomposition of the state $|\Uparrow\rangle + |\Downarrow\rangle$ for a split at $M/2$ from its matrix product representation for OBC. Explain the connection between properties of the matrices C and the amount of entanglement in $|\Uparrow\rangle + |\Downarrow\rangle$.

(iv) Determine a matrix product representation of the anti-ferromagnetic superposition state $|\uparrow\downarrow\cdots\uparrow\downarrow\rangle + |\downarrow\uparrow\cdots\downarrow\uparrow\rangle$ using PBC.

(v) The W-state is an equal superposition of all translates of states $|\downarrow\uparrow\cdots\uparrow\rangle$. In contrast to the previous examples, despite this state possessing full permutation symmetry, there is no translationally invariant matrix product representation of a W-state with 2×2 matrices for all sites m and PBC. Instead the simplest representation of a W-state uses OBC and does not fully share its symmetries. Show that the choice

$$A^{\uparrow} = I \ , \ A^{\downarrow} = \sigma^{+}$$

realizes the W-state for boundary states $|\Phi_0\rangle = |\uparrow\rangle$ and $|\Phi_M\rangle = |\downarrow\rangle$. Is this a canonical form of matrix product state?

(vi) Show that the three body Hamiltonian

$$H = \sum_m \sigma^z_m \sigma^x_{m+1} \sigma^z_{m+2} \ ,$$

with PBC has a matrix product state with matrices

$$A^{\uparrow} = \sigma^{-} + \frac{1}{2}(1-\sigma^z) \ , \qquad A^{\downarrow} = \frac{1}{2}(1+\sigma^z) - \sigma^{+} \ ,$$

as its ground state. There is no need to show that this ground state is unique.

3. **Correlation functions of matrix product states**

Let us consider an MPS which is translationally invariant, i.e. the matrices A are site independent and PBC. We assume for simplicity (this is not necessarily always true but the conclusions will still hold) that the transfer matrix can be diagonalized and has one eigenvalue $\nu_1 = 1$ while all other eigenvalues ν_γ with $\gamma = 2\cdots\chi^2$ have a modulus smaller than 1 and are arranged in descending order. The corresponding right and left eigenvectors are $|r_\gamma\rangle$ and $|l_\gamma\rangle$. We are interested in correlation functions of the form $C_l = \langle O_l O_m\rangle - \langle O_l\rangle\langle O_m\rangle$. Show that these can be written as

$$C_l = \sum_{\gamma=2}^{\chi^2} \kappa_\gamma \left(\frac{\nu_\gamma}{|\nu_\gamma|}\right)^l e^{-l/\xi_\gamma} \ ,$$

and calculate the parameters κ_γ and ξ_ν appearing in this expression. Conclude that MPS do not well approximate quantum systems with power law correlation functions when $l \to \infty$.