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.

Solution: This state is an MPS with $\chi = 1$ and 1×1 matrices $A_m^n = f_n^{(m)}$.

(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.

Solution: The energy expectation value is given by

$$E = \langle G|\,H\,|G\rangle = M\sum_n\left(\frac{U}{2}n(n-1) - \mu n\right) f_n^2$$

and we have set $f_n^{(m)} = f_n = |f_n|$. We search for the minimum of E subject to the constraint $\sum_n f_n^2 = 1$. The bracket has one global minimum at

$$n = \bar{n} = \frac{1}{2} + \frac{\mu}{U} \ .$$

Thus the vacuum state with $f_n = \delta_{n,0}$ will be the ground state for $\bar{n} \le 0$ and the energy will be minimized by MI states $f_n = \delta_{n,n_0}$. For finding n_0 we need to calculate the ratio of μ/U for which it becomes energetically favorable to go from $n_0 \to n_0 + 1$. This happens when

$$\frac{U}{2}n_0(n_0-1) - \mu n_0 = \frac{U}{2}(n_0+1)n_0 - \mu(n_0+1) ,$$

and thus at $n_0 = \mu/U$. The ground state therefore is given by the MI state with $n_0 = [1+\mu/U]$ where [] denotes the largest integer. We find $\langle G|\,a_m^\dagger a_m a_m^\dagger a_m\,|G\rangle = n_0^2$ and $\langle G|\,a_m^\dagger a_m\,|G\rangle^2 = n_0^2$ and therefore the particle number fluctuations are zero.

(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

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

Solution: The normalization factor is $\mathcal{N} = (1+2\epsilon)^{-M/2}$. The total number of particles is

$$\bar{N} = M(\epsilon \times 0 + 1 \times 1 + \epsilon \times 2)^2 \mathcal{N}^2 = M \ ,$$

which is independent of ϵ and the same as for the $n_0 = 1$ MI state. We work out the expectation values

$$\langle a_m \rangle = \frac{\sqrt{\epsilon}(1+\sqrt{2})}{1+2\epsilon} \ ,$$

and find

$$\left\langle a_m^\dagger a_m a_m^\dagger a_m \right\rangle = \frac{1+4\epsilon}{1+2\epsilon} \ .$$

The total energy of the system is thus given by

$$E_\epsilon = \langle G_\epsilon | H | G_\epsilon \rangle = M \left(-2J\epsilon \left(\frac{1+\sqrt{2}}{1+2\epsilon} \right)^2 + \frac{U}{2}\frac{1+4\epsilon}{1+2\epsilon} - \frac{U}{2} - \mu \right) \ .$$

We expand this expression to first order in ϵ and find

$$E_\epsilon = M\epsilon(-2J(1+\sqrt{2})^2 + U) + \text{const.} + \mathcal{O}(\epsilon^2) \ .$$

The MI state will thus be unstable for

$$\left(\frac{U}{2J} \right) < \left(\frac{U}{2J} \right)_{crit} = (1+\sqrt{2})^2 \approx 5.8.$$

(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.

Solution: This is a coherent state whose coefficients (including normalization) are given by

$$f_n^{(m)} = e^{-\frac{|\phi_m|^2}{2}} \frac{\phi_m^n}{\sqrt{n!}} \ .$$

It has the properties $a_m |G\rangle = \phi_m |G\rangle$ and $\left| \dot{G} \right\rangle = \sum_m a_m^\dagger \dot{\phi}_m |G\rangle$ which we use to derive Euler-Lagrange equations which minimize $\langle G| \mathrm{i}\partial_t - H |G\rangle$. These are given by the set of equations

$$\mathrm{i}\dot{\phi}_m = -J(\phi_{m+1} + \phi_{m-1}) + U|\phi_m|^2\phi_m - \mu\phi_m \ ,$$

and a trap potential can easily be accounted for by making μ space dependent. We identify the macroscopic wave function $\Psi(x)\sqrt{\ell} = \phi_m$ at the discrete points $x = m\ell$ where $\ell = \lambda/2$ is the lattice period. A discretized version of the second derivative of the wave function is

$$\Psi''(m\ell) = \frac{\phi_{m+1} - 2\phi_m + \phi_{m-1}}{\ell^{5/2}} \ ,$$

and we can rewrite the evolution equation as

$$\mathrm{i}\dot{\Psi}(x) = -J(\Psi''(x)\ell^2 + 2\Psi(x)) + U\ell|\Psi(x)|^2\Psi(x) - \mu\Psi(x) \ .$$

This corresponds to a Gross Pitaevskii equation with effective mass $m_{\text{eff}} = 1/2J\ell^2$ and $g = U\ell$. We find $\langle G| a_m^\dagger a_m a_m^\dagger a_m |G\rangle = |\phi_m|^2(|\phi_m|^2 + 1)$ and $\langle G| a_m^\dagger a_m |G\rangle^2 = |\phi_m|^4$ and therefore the variance in the particle number in each site is $|\phi_m|^2$.

(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?

Solution: Briefly: Any Gutzwiller state other than an MI state violates particle number conservation. The macroscopic wave function does not contain correlations between different positions, i.e. all local observables are uncorrelated with other parts of the condensate. This is identical to what happens in the Gutzwiller approximation.

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.

Solution: We have $A_m^\uparrow = B_m^\downarrow = 1$ and $B_m^\uparrow = A_m^\downarrow = 0$. When using OBC all boundary states are 1.

(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).

Solution: The direct sum yields $C_m^\uparrow = (I + \sigma^z)/2 = |\uparrow\rangle\langle\uparrow|$ and $C_m^\downarrow = (I - \sigma^z)/2 = |\downarrow\rangle\langle\downarrow|$. Their products are $(C^\uparrow)^n = C^\uparrow$ and $(C^\downarrow)^n = C^\downarrow$, while $C^\uparrow C^\downarrow = C^\downarrow C^\uparrow = 0$. The trace of the matrix product will thus be 1 if all spins are aligned and 0 otherwise. Suitable boundary states for OBC are $|\Phi_0\rangle = (1,1)'$ and $|\Phi_M\rangle = (1,1)'$. The matrices fulfill the conditions of canonical MPS.

(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 $|\Uparrow\rangle + |\Downarrow\rangle$.

Solution: The diagonal matrix has two degenerate eigenvalues of 1 (Note: the state is not normalized, otherwise the eigenvalues would be $1/\sqrt{2}$). The resolution of I in terms of the the corresponding eigenvectors is $I = |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|$ and therefore we find

$$|\Uparrow\rangle + |\Downarrow\rangle = 1\left|\uparrow_1 \cdots \uparrow_{M/2}\right\rangle \otimes \left|\uparrow_{M/2+1} \cdots \uparrow_M\right\rangle + 1\left|\downarrow_1 \cdots \downarrow_{M/2}\right\rangle \otimes \left|\downarrow_{M/2+1} \cdots \downarrow_M\right\rangle \ ,$$

as expected.

(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.

Solution: The MPS of $|\uparrow\downarrow\cdots\rangle$ is given by $A_{\text{odd}}^\uparrow = 1$, $A_{\text{even}}^\uparrow = 0$, $A_{\text{odd}}^\downarrow = 0$, $A_{\text{even}}^\downarrow = 1$. The MPS of $|\downarrow\uparrow\cdots\rangle$ is given by $A_{\text{odd}}^\uparrow = 0$, $A_{\text{even}}^\uparrow = 1$, $A_{\text{odd}}^\downarrow = 1$, $A_{\text{even}}^\downarrow = 0$. From the result in (ii) we thus find the the superposition state MPS is given by $C_{\text{odd}}^\uparrow = C_{\text{even}}^\downarrow = (I + \sigma^z)/2$ $C_{\text{even}}^\uparrow = C_{\text{odd}}^\downarrow = (I - \sigma^z)/2$. This is not translationally invariant but the state is. The main property of these matrices is $C_{\text{odd}}^\uparrow C_{\text{even}}^\uparrow = 0$, $C_{\text{odd}}^\downarrow C_{\text{even}}^\downarrow = 0$ and $C_{\text{odd}}^\uparrow C_{\text{even}}^\downarrow = |\uparrow\rangle\langle\uparrow|$, $C_{\text{odd}}^\downarrow C_{\text{even}}^\uparrow = |\downarrow\rangle\langle\downarrow|$. This can also be achieved by the translationally invariant matrices (M even) $C^\uparrow = |\uparrow\rangle\langle\downarrow|$ and $C^\downarrow = |\downarrow\rangle\langle\uparrow|$.

(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?

Solution: If all spins are up the matrix product is $\langle\uparrow|\,I\,|\downarrow\rangle = 0$. If one spin is down the matrix product is given by $\langle\uparrow|\,|\uparrow\rangle\,\langle\downarrow|\,|\downarrow\rangle = I$ with a trace of 2. Since $(A^{\downarrow})^2 = 0$ the trace will be zero whenever more than one spin is down. The matrices fulfil all conditions for this MPS to be canonical.

(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.

Solution: The matrices E are given by

$$E^{\uparrow\uparrow} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \end{pmatrix}\ , \qquad E^{\uparrow\downarrow} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$E^{\downarrow\uparrow} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\ , \qquad E^{\downarrow\downarrow} = \begin{pmatrix} 1 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\ .$$

We have $O^z = E^{\uparrow\uparrow} - E^{\downarrow\downarrow}$, $O^x = E^{\uparrow\downarrow} + E^{\downarrow\uparrow}$ and $\mathcal{I} = E^{\uparrow\uparrow} + E^{\downarrow\downarrow}$. We find

$$\mathcal{I}^n = 2^{n-1} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}\ .$$

The product $O^z O^x O^z = -\mathcal{I}^3$. We therefore find for the energy E of this state

$$E = M\frac{\mathrm{tr}\left\{\mathcal{I}^{M-3} O^z O^x O^z\right\}}{\mathrm{tr}\left\{\mathcal{I}^M\right\}} = -M\ .$$

Each of the M term in H is bounded by -1 and thus the state is a ground state. The state is the unique ground state as can e.g. be shown by using the stabilizer formalism.

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 $l \to \infty$.

Solution: We write $\mathcal{I} = \sum_\gamma \nu_\gamma |r_\gamma\rangle \langle l_\gamma|$ with $\langle l_\gamma | r_{\gamma'} \rangle = \delta_{\gamma,\gamma'}$. For $M \to \infty$ we have $\mathcal{I}^M = |r_1\rangle \langle l_1|$ and

$$C_l = \langle O_m O_{m+l} \rangle - \langle O_m \rangle \langle O_{m+l} \rangle = \mathrm{tr} \left\{ O \mathcal{I}^{l-1} O \mathcal{I}^{M-l-1} \right\} - \left(\mathrm{tr} \left\{ O \mathcal{I}^{M-1} \right\} \right)^2 \ .$$

We rewrite this as

$$C_l = \sum_\gamma \langle l_1| O \nu_\gamma^{l-1} |r_\gamma\rangle \langle l_\gamma| O |r_1\rangle - (\langle r_1| O |l_1\rangle)^2 = \sum_{\gamma=2}^{\chi^2} \nu_\gamma^{l-1} \langle l_1| O |r_\gamma\rangle \langle l_\gamma| O |r_1\rangle \ ,$$

and thus we find $\kappa_\gamma = \langle l_1| O |r_\gamma\rangle \langle l_\gamma| O |r_1\rangle / \nu_\gamma$ and the correlation lengths $\xi_\gamma = 1/\ln |\nu_\gamma|$.