Master ICFP

Ultracold Atoms

Exercise class n°9: Particle-hole excitations in a bosonic Mott insulator

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Bosonic atoms in optical lattices feature the superfluid to Mott insulator transition upon increasing the strength of interactions. A qualitative description of the transition was derived in the lectures using a variational approach, based on Gutzwiller wavefunctions. The latter consist in products of on-site wavefunctions; it thus neglects correlations between lattice sites.

We discuss here a perturbative approach valid in the limit of strong interactions, which will reveal short-range correlations in the Mott insulating phase induced by the tunnel coupling.

We remind the expression of the Bose-Hubbard Hamiltonian

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \sum_i \frac{U}{2} \hat{n}_i(\hat{n}_i + 1) - \mu \hat{n}_i.$$

For simplicity we restrict the discussion to a one-dimensional system. The lattice period is denoted d.

1. Let us first consider the ground state $|\psi_0\rangle$ for $J = 0$. Show that it can be written as

$$|\Psi_0\rangle = \prod_i |n_0\rangle_i \,,$$

   where $|n_0\rangle_i$ is the state with n_0 particles in the site i. What is the value of n_0 as a function of the chemical potential μ?

We assume in the following that the chemical potential is chosen such that $n_0 > 0$. We now consider the effect of a small tunnel coupling $J \ll U$.

2. Using first-order perturbation theory, show that the ground state can be written as

$$|\Psi\rangle \simeq |\Psi_0\rangle + \frac{J}{U} \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j \, |\Psi_0\rangle \,.$$

We define quantum states $|p : i, h : j\rangle$ as a particle-hole state, with $n_0 + 1$ particles at the site i, $n_0 - 1$ particles at j, and n_0 particles elsewhere.

3. Show that the ground state can be written as

$$|\Psi\rangle \simeq |\Psi_0\rangle + \frac{J}{U} \sum_{\langle i,j \rangle} \sqrt{n_0(n_0+1)} \, |p : i, h : j\rangle \,.$$

4. Calculate the value of the discrete first-order correlation function, defined as

$$C_1(i,j) = \langle \Psi | \, \hat{a}_i^\dagger \hat{a}_j \, |\Psi\rangle \,.$$

5. Explain why calculating the correlation between sites separated by n links requires to push the perturbation expansion up to order n at least.

We thus expect the following scaling for the correlation function:

$$C_1(i,j) \sim \left(\frac{J}{U}\right)^{|i-j|}. \tag{1}$$

We also introduce the real-space correlation function $G_1(x,x') = \langle\Psi|\,\hat{\psi}^\dagger(x)\hat{\psi}(x')\,|\Psi\rangle$, where $\hat{\psi}(x)$ is the field operator.

6. Show that the real-space and discrete correlation functions are related by

$$G_1(x,x') = \sum_{i,j} w(x-id)^* w(x-jd) C_1(i,j),$$

where $w(x)$ is the Wannier function centered on the site $i=0$.

7. A crude estimate of g_1 can be obtained by assuming that $w(x)$ vanishes outside the site 0 (i.e. $w(x)=0$ for $|x|>a/2$). Using eq. (**??**), show that we expect the scaling

$$G_1(x,x') \sim e^{-|x-x'|/\xi}$$

at large distances, and give the value of the correlation length ξ.

8. What is the value of the correlation length ξ, defined as $g_1(x,x') \sim e^{-|x-x'|/\xi}$?

We remind the connection between the momentum distribution and the correlation function

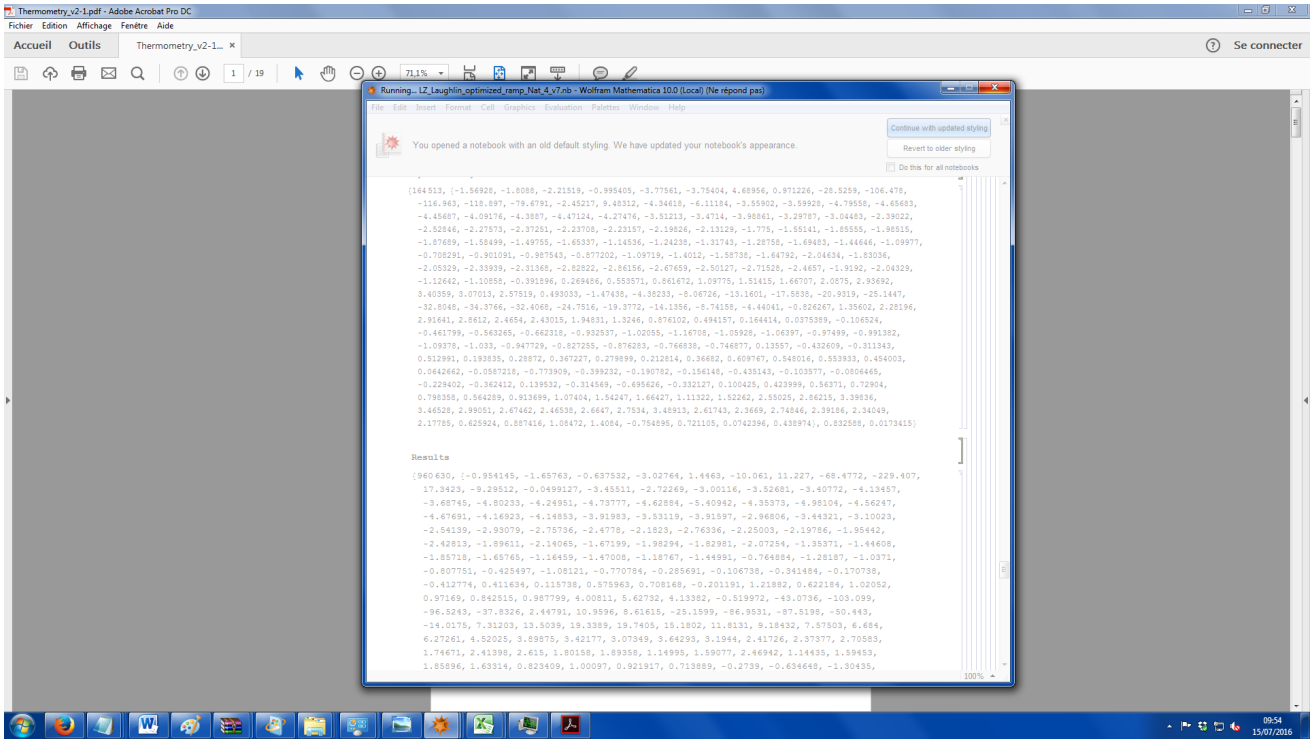
$$n(k) = \frac{1}{N}|\tilde{w}(k)|^2 \sum_{i,j} e^{ikd(i-j)} C_1(i,j),$$

where $\tilde{w}(k)$ is the Wannier function in momentum space and N is the number of lattice sites.

9. Calculate the momentum distribution using the ground state obteined using first-order perturbation theory, and show that it can be written as

$$n(k) = |\tilde{w}(k)|^2 \left[n_0 + \frac{4Jn_0(n_0+1)}{U}\cos(kd)\right].$$

The modulation $\propto \cos(kd)$ reveals the coherence within the Mott insulating phase. It was measured experimentally using a 3D system, by measuring the 'visibility' of the interference pattern measured after time of flight.


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