Short-range coherence of a lattice Bose atom gas in the Mott insulating phase

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We study the short-range coherence of ultracold lattice Bose gases in the Mott insulating phase. We calculate the visibility of the interference pattern and the results agree quantitatively with the recent experimental measurement (Phys. Rev. Lett. 95, 050404 (2005)). The visibility deviation from the inversely linear dependence on the bare on-site interaction $U_0$ is explained both in smaller and larger $U_0$. For a smaller $U_0$, it comes from a second order correction. For a larger $U_0$, except the breakdown of adiabaticity as analyzed by Gerbier et al, there might be another source to cause this deviation, which is the diversity between $U_0$ determined by the single atom Wannier function and the effective on site interaction $U_{\text{eff}}$ for a multi-occupation per site.

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The observation of the Mott insulating phase in ultracold Bose gases in an optical lattice opens a new era to investigate exactly controllable strong-correlated systems for a one-component lattice Bose gases, the Bose Hubbard model captures the basic physics of the systems. The theoretical studies mostly focused on the sharp phase transition between the superfluid/Mott insulator transition. The result is exactly the same as obtained by Gerbier et al by assuming a small admixture of particle-hole pairs in the ground state of the Mott insulating phase. They showed that the visibility of interference pattern calculated by this ground state may well match the experimental data in a wide intermediate range of $U_0$.

There were deviations from the inverse linear power law in both small and large $U$ in the measurement of the visibility. Gerbier et al interpreted the large $U$ deviation is caused by a breakdown of adiabaticity since the ramping time used in the experiment has been close to the tunnelling time. For the deviation in a small $U$, there was no explanation yet.

In this paper, we will analytically prove the inverse linear power law of the visibility for intermediate $U$ in the zero temperature. Here the words 'intermediate $U$' (as well as 'small $U$', 'large $U$' in this work) mean the magnitude of $U - U_c$ is intermediate (small or large), with $U_c$ the critical interaction strength of the superfluid/Mott insulator transition. The result is exactly the same as that obtained by Gerbier et al by assuming a small admixture of the particle hole pair in the ground state. We also show the deviation of the visibility from the inverse linear power law in a small $U$ is caused by a second order correction. For the large $U$, we show that, except the explanation by the authors of the experimental work, owing to the multi-occupation per site, the effective on-site interaction $U_{\text{eff}}$ which appears in the Bose Hubbard model is different from $U_0$ which was determined by the single atom Wannier function and used to fit the data of the experiment.

We consider a one-component Bose gas in a 3-dimensional optical lattice described by a periodic potential $V_0(\vec{r})$. Although the real experimental system was confined by a trap potential, we here only pay our attention to the homogeneous system. Beginning with the expansion of the boson field operators in a set of localized basis, i.e., $\psi(\vec{r}) = \sum a_i w(\vec{r} - \vec{r}_i)$ and keeping only the lowest vibrational state, one can define an on-site free energy $f = n I + U n (\bar{n} - 1)/2$, where $\bar{n}$ is the average occupation per site. The on-site energy $I$ and the bare on-site interaction $U$ are defined by

$$I = \int d\vec{r} w^*(\vec{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_0(\vec{r}) \right] w(\vec{r}),$$

$$U = \frac{4\pi a_s \hbar^2}{m} \int d\vec{r} |w(\vec{r})|^4.$$  

This on-site free energy contributes to the chemical potential by $\mu = -\partial f/\partial \bar{n}$ and defines the effective on-site interaction

$$U_{\text{eff}} = \partial^2 f/\partial \bar{n}^2.$$  

For the single occupation per site, $U_{\text{eff}} = U = U_0$ and the difference appears for $\bar{n} > 1$. We will be back to this issue later. The Bose Hubbard model for a homogeneous lattice gases is defined by the following Hamiltonian

$$H = -t \sum_{\langle ij \rangle} a_i^\dagger a_j + \frac{U_{\text{eff}}}{2} \sum_i a_i^\dagger a_i a_i^\dagger a_i - \mu \sum_i a_i^\dagger a_i,$$

where $\langle ij \rangle$ denotes the sum over the nearest neighbor sites and $\mu$ is the chemical potential. The tunnelling amplitude is defined by

$$t_{B,F;ij} = \int d\vec{r}^* w^*(\vec{r} + \vec{r}_i) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_0(\vec{r}) \right] w(\vec{r} + \vec{r}_j),$$

for a pair of the nearest neighbor sites $(i, j)$. [12]
Our main goal is to calculate the interference pattern
\[
S(\vec{k}) = \frac{1}{\beta} \sum_{i,j} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)} \langle a_i^{\dagger} a_j \rangle, \tag{4}
\]
which is related to the density distribution of the expanding atom clouds by \( \rho(\vec{r}) = \frac{m}{\hbar^2} |w(\vec{r}) = m\vec{r}/\hbar t_{\text{res}}|^2 S(\vec{k}) \) with \( m \) the atom mass and \( t_{\text{res}} \) the time of the atom free expansion \[12, 18\]. Since we are interested in the Mott tunneling term as a perturbation. To do this, we introduce a Hubbard-Stratonovich field in the partition function \[7,9\]
\[
Z[J, J^*] = \int \mathcal{D} \Phi^* \mathcal{D} \Phi \mathcal{D} a^\dagger \mathcal{D} a \exp \left\{ -S_0 + t \int \frac{d\tau}{\beta} \sum_{\langle ij \rangle} a_i^\dagger a_j + \int \frac{d\tau}{\beta} \sum_i (J_i^* a_i + J_i a_i^\dagger) - t \int \frac{d\tau}{\beta} (a_i^\dagger - \Phi_i^* + J_i^*/t)(a_j - \Phi_j + J_j/t) \right\}, \tag{5}
\]
where \( S_0 \) is the \( t \)-independent part in the full action and \( J \) and \( J^* \) are currents introduced to calculate correlation functions. Integrating away \( a_i \) and \( a_i^\dagger \) and transferring into the lattice wave vector and thermal space frequency, one has
\[
Z[J^*, J] = \int \mathcal{D} \Phi^* \mathcal{D} \Phi \exp \left\{ \sum_{\vec{k}, n} (-\Phi_{\vec{k}, n} G^{-1}(\vec{k}, i\omega_n) \Phi_{\vec{k}, n}^\dagger + J_{\vec{k}, n} \Phi_{\vec{k}, n} + J_{\vec{k}, n}^* \Phi_{\vec{k}, n}^\dagger + 1/\epsilon_k J_{\vec{k}, n} J_{\vec{k}, n}^*) \right\}, \tag{6}
\]
where \( \epsilon_k = -2t \sum_{\alpha=x,y,z} \cos k_\alpha \). The correlation function is calculated in a standard way:
\[
\langle a_{\vec{k}, n}^\dagger a_{\vec{k}, n} \rangle = \frac{1}{Z[0,0]} \frac{\delta^2 Z[J^*, J]}{\delta J_{\vec{k}, n} \delta J_{\vec{k}, n}^*} \bigg|_{J^* = J = 0} = \langle \Phi_{\vec{k}, n}^\dagger \Phi_{\vec{k}, n} \rangle + 1/\epsilon_k = -G^{-1}(\vec{k}, i\omega_n) + 1/\epsilon_k. \tag{7}
\]
The interference pattern then may be expressed as
\[
S(\vec{k}) = \frac{1}{\beta} \sum_n \left[ G(\vec{k}, i\omega_n) - 1/\epsilon_k \right]. \tag{8}
\]
In the Mott insulating phase, the correlation function \( G(\vec{k}, i\omega_n) \) has been calculated by slave particle techniques \[5,9\]
\[
G^{-1}(\vec{k}, i\omega_n) = \epsilon_k - 2t \sum_{\alpha=0}^{\infty} (\alpha + 1) \frac{n^\alpha - n^{\alpha+1}}{\omega_n + \mu - \alpha U}, \tag{9}
\]
where the slave particle occupation number is given by
\[
n^\alpha = \frac{1}{\exp[\beta(-i\lambda - \alpha \mu + \alpha(\alpha - 1)U/2)] + 1} \tag{10}
\]
which obeys \( \sum_\alpha n^\alpha = 1 \) and \( \sum_\alpha \alpha n^\alpha = N \) in the mean field approximation \[12\]. \( \lambda \) is a Lagrangian multiplier to ensure \( \sum_\alpha n^\alpha = 1 \). The sign \( \pm \) corresponds to the slave fermion or boson, respectively. In previous works, we have show that the slave fermion approach may have some advantages to the slave boson approach \[3,10\]. We then take the slave fermion formalism. In the Mott insulating phase, since \( U_{\text{eff}} \gg t \), one can expand \( G(\vec{k}, i\omega_n) \) in terms of \( \epsilon_k/(i\omega_n - \mu + \alpha U_{\text{eff}}) \) and the interference pattern reads
\[
S(\vec{k}) = \frac{1}{\beta} \sum_n \left[ G(\vec{k}, i\omega_n) - 1/\epsilon_k \right] = \frac{1}{\beta} \sum_n \sum_{\alpha=0}^{\infty} (-1)^\alpha \epsilon_k^\alpha (A(\omega_n))^\alpha + 1, \tag{11}
\]
\[
A(\omega_n) = \sum_{\alpha=0}^{\infty} (\alpha + 1) n^{\alpha+1} - n^\alpha \approx \omega_n + \mu - \alpha U_{\text{eff}}. \tag{12}
\]
Making the frequency sum, one has, to the first order of \( \epsilon_k \),
\[
S(\vec{k}) \approx -\sum_\alpha n_B(\alpha U_{\text{eff}} - \mu)(\alpha + 1)(n^{\alpha+1} - n^\alpha) - \epsilon_k \beta \sum_\alpha [(\alpha + 1)^2 (n^{\alpha+1} - n^\alpha)^2 - \epsilon_k^2 U_{\text{eff}}] (n_B(\alpha U_{\text{eff}} - \mu)(1 + n_B(\alpha U_{\text{eff}} - \mu)) - 2 \epsilon_k U_{\text{eff}} \sum_{\alpha<\gamma} (n_B(\alpha U_{\text{eff}} - \mu) - n_B(\gamma U_{\text{eff}} - \mu)) \times (\alpha + 1)(\gamma + 1)(n^{\alpha+1} - n^\alpha)(n^{\gamma+1} - n^\gamma), \tag{13}
\]
where \( n_B(\alpha U_{\text{eff}} - \mu) = [e^{\beta(\alpha U_{\text{eff}} - \mu)} - 1]^{-1}. \) In the limit \( T \rightarrow 0 \) and the \( n_0 \)-th Mott lobe, one knows \( (n_0 - 1) U_{\text{eff}} < \mu < n_0 U_{\text{eff}} \), \( n^\alpha = \delta_{\alpha,n_0}. \) Substituting these into \[12\], one obtains the zero temperature value of \( S(\vec{k}) \)
\[
S(\vec{k}, T = 0) = n_0 - 2n_0(n_0 + 1) \frac{\epsilon_k}{U_{\text{eff}}}. \tag{14}
\]
This is what Gerber et al obtained by assuming the particle-hole pair admixture in the ground state \[13\]. Integrating along one lattice direction, the corresponding 2D visibility is given by
\[
\nu = \frac{\rho_{\max} - \rho_{\min}}{\rho_{\max} + \rho_{\min}} = \frac{S_{\max} - S_{\min}}{S_{\max} + S_{\min}} \approx \frac{4}{3} (n_0 + 1) L U_{\text{eff}} \tag{15}
\]
for \( z = 6 \), where \( \rho_{\max} \) and \( \rho_{\min} \) are chosen such that the Wannier envelop was cancelled. This is the inverse linear power law used to fit the experimental data \[13\]. However, the experimental data deviated from this power law fit when \( U_{\text{eff}}/zt < 8 \). In terms of \[11\], we think that this comes from a second order correction. A direct calculation shows that the second order correction in zero temperature is given by \[20\]
\[
\delta^{(2)} S(\vec{k}) = 3n_0(n_0 + 1) \frac{\epsilon_k^2}{U_{\text{eff}}^2}. \tag{16}
\]
Thus, the 2D visibility for \( n_0 = 1 \) is modified to
\[
\nu = \frac{8}{3U_{\text{eff}}(1 + 32U_{\text{eff}}^2/3)} \tag{17}
\]
with $\bar{U}_{\text{eff}} = U_{\text{eff}}/zt$. In Fig. 1 we show the visibility against $\bar{U}_{\text{eff}}$ in a log-log plot for $n_0 = 1$. This second order correction suppresses the visibility for a small $\bar{U}_{\text{eff}}$ whereas the exponent of the power law seems deviating from $-1$ a little. These features agree with the experimentally measured data.

![FIG. 1: Visibility of the interference pattern versus $\bar{U}_{\text{eff}}$ according to (16) in a log-log plot (the dot line with circles). The solid line is the inverse linear power law (13) and the dash line is a power law fit with an exponent $-0.95$ to (16).](image)

We have neglected the finite temperature effect to compare with the experiment although our theory is in finite temperature. In fact, there may be a finite temperature correction to the interference pattern in the second order. According to (11), it is given by, near $n_0 = 1$

$$\delta^{(2)} S_T(\hat{k}) = 18(n^2)^2 \frac{\epsilon^2}{U_{\text{eff}}^2},$$

(17)

which may further suppresses the visibility. For instance, at $T = 1.0zt \sim 10^4\text{nK}$, the ratio between (17) and (16) is

$$\frac{\delta_T^{(2)} S(\hat{k})}{\delta^{(2)} S(k)} = 3(n^2)^2 n^2 / 2$$

$$= 0.106, 0.098, 0.087, \text{ and } 0.064$$

for $\bar{U}_{\text{eff}} = 6, 7, 8, \text{ and } 10$. However, the temperature in the Mott insulator is difficult to be estimated in the experiment [22]. Thus, a quantitative comparison of the finite temperature calculation to the experiment data is waiting for more experimental developments.

We now discuss the large $U$ deviation from the inverse linear power law, which has been seen in the experiment and explained by the breakdown of adiabaticity [13]. We will reveal another possible source for this deviation. As we have mentioned before, the value of $U_{\text{eff}}$ may be different from $U$ and $U_0$ for $\bar{n} > 1$. Our above calculation showed an inverse linear power law to $U_{\text{eff}}$ whereas the experimentalists used $U_0$ to fit their data.

![FIG. 2: (Color online) The effective on-site interaction $U_{\text{eff}}$ versus the average occupation per site, $\bar{n}$ in a $\bar{n}$-log($U_{\text{eff}}$) plot. The thin solid lines are linear fits to variational data for $V_0 = 11.95, 14.32, 16.25 \text{ and } 29 \text{ } E_R$ (empty circles, filled triangles, empty triangles and filled circles, respectively). The dash line is critical interaction strength calculated by the mean field theory [16]. The thick horizontal lines are the on-site interactions $U_0$ calculated by the single atom Warrier function.](image)

Due to the interaction, the atom energy band may be modified and the Wannier function may be broadened, compared to the single atom ones. In Ref. [17], we have considered the mean field interaction and made a variational calculation to the Wannier function by using Kohn’s method [21]. The direct result of the broadening of the Wannier function is the bare on-site interaction $U$ becomes weaker than $U_0$ which is calculated by the single atom Wannier function. The $\bar{n}$-dependence of $I$ may further reduce $U_{\text{eff}}$ from $U$. In Fig. 2 we plot $U_{\text{eff}}$ versus $\bar{n}$. In the low part of Fig. 2, three typical lattice depths are considered, $V_0 = 11.95, 14.32$ and $16.25 \text{ } E_R(= \frac{k^2 \xi^2}{2m})$, corresponding to the critical interaction strengths of the $n_0 = 1, 2$ and $3$ Mott states. The up-part is for $V_0 = 29 \text{ } E_R$, which was the lattice depth where the adiabaticity breaks [16].

Several points may be seen from Fig. 2. First, the critical values of $V_0 = 14.32 \text{ } E_R$ for $n_0 = 2$ and $16.25 \text{ } E_R$ for $n_0 = 3$ are closer to experimental ones, $14.1(8) \text{ } E_R$ and $16.6(9) \text{ } E_R$, comparing to $14.7 \text{ } E_R$ and $15.9 \text{ } E_R$, corresponding to the single atom Wannier functions. Second, the variational data are downward as $\bar{n}$ indicates that $-\log U_{\text{eff}} > -\log U_0$ for $\bar{n} > 1$. This may cause two results: (a) If $-\log U_{\text{eff}}$ deviates from $-\log U_0$ a small magnitude, the power law fit presents an exponents $-(1 - \delta)$. This has been observed in experiment, which is $-0.98(7)$ [13]. (b) As $\bar{n}$ increases, the deviation becomes significant. This may appear in a large $V_0$. In the experiment, the latter appeared in $V_0 > 29 \text{ } E_R$. We show that, in Fig. 2 the deviation is not a small magnitude for $V_0 = 29 \text{ } E_R$.

In summary, we studied the short-range coherence in the Mott insulating phase with a finite on-site interaction strength. The interference pattern and then its visibility were calculated by using a perturbation theory. The inverse linear power law of the visibility to the interaction strength, which was found in the experiment, was exactly
recovered. We further discussed the deviation from this power law both in a small and large $U_0$. We found that a second order effect suppresses the visibility for a small $U_0$ while its up-deviation in a large $U_0$ might be caused by the difference between $U_0$ and $U_{\text{eff}}$ except the possible breakdown of adiabaticity.

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