Density fluctuations of a hard-core Bose gas in a one-dimensional lattice

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For a hard-core Bose gas on a one-dimensional lattice we find characteristic oscillations in the density-density correlation function. Their wavelength diverges as the system undergoes a continuous transition from an incommensurate to a Mott insulating phase. The associated static structure factor vanishes as the Mott insulating phase is approached. The qualitative picture is unchanged when a weak confining potential is applied to the system.

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Recent experiments on one-dimensional (1D) Bose systems [1, 2, 3] have opened an exciting new field of physics. This will provide us with an extended and deeper understanding of the special properties of strongly interacting particles at low dimensions. From the theoretical point of view 1D systems are easier to treat in comparison with two- and three-dimensional systems but also prevent us from using conventional mean-field methods.

A well-known fact of one-dimensional many-body physics is that a hard-core Bose gas is equivalent to a free Fermi gas [4, 5]. The role of the hard-core interaction of bosons is played by the statistical properties of the fermions, related to Pauli’s principle. This idea can be conveyed to 1D lattice systems.

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For directed polymers in two dimensions it was shown that Z can be expressed as a determinant [6]. Thus the partition function of hard-core bosons in d = 1 reads

\[ Z = \det R, \]

where R is diagonal with respect to the Matsubara frequency \( \omega \)

\[ R(\omega) = (e^{i\omega} - \zeta^{-1})\sigma_0 + \frac{J}{2}(1 + e^{i\omega} + \hat{T}^{-1} + e^{i\omega}\hat{T})\sigma_1 - \frac{i}{2}(1 - e^{i\omega} + \hat{T}^{-1} - e^{i\omega}\hat{T})\sigma_2. \]

\( \hat{T} \) is the shift operator along the 1D lattice (\( \hat{T} f(r) = f(r + 1) \)), and the \( \sigma_j \) are the Pauli matrices

\[ \sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \]

This model describes the tunneling of bosons with rate \( J \geq 0 \) between nearest neighbors, expressed by the shift operator \( \hat{T} \) and its inverse \( \hat{T}^{-1} \). \( J \) is measured in units of the lattice potential. The 2 \( \times \) 2 structure arises from the fact that particle exchange between neighboring sites through simultaneous tunneling is prohibited. This reduces the translational symmetry to sublattices with every second site, where \( r \) is the position on a sublattice. \( \zeta > 0 \) is the fugacity that controls the density of bosons in the system. The fugacity is not directly accessible in the experiment but only indirectly through the density \( n(\zeta, J) \). Therefore, physical quantities should be measured as functions of \( n \) and \( J \). An additional potential, superimposed on the optical lattice, is described by a space-dependent fugacity \( \zeta_r \).

Physical quantities can be derived from the matrix R. For instance, if we are interested in properties at zero temperature we can use the integral with respect to the Matsubara frequency

\[ G_{r,r'} = \int_0^{2\pi} (R^{-1})_{r,r'} \frac{d\omega}{2\pi} \]

to evaluate the local density of bosons as

\[ n_r = 1 + \zeta_r^{-1} G_{r,r} . \]

It should be noticed that \( G_{r,r'} \) is not the Green’s function for the propagation of an individual boson in the system but a correlation function between two bosons. Therefore, it is not possible to evaluate the momentum distribution of bosons \( n\{k\} \) from this expression. On the other hand, the evaluation of the density and the density-density correlation function becomes a simple task with the matrix \( G_{r,r'} \).

Another interesting quantity is the correlation function of the density fluctuations

\[ C_{r,r'} \equiv -\langle (n_r - \langle n_r \rangle) (n_{r'} - \langle n_{r'} \rangle) \rangle = (\zeta_r \zeta_r')^{-1} G_{r,r'} G_{r',r} \]

from which the static structure factor as a function of the momentum \( k \) can be obtained by Fourier transformation:

\[ S_k = \frac{1}{N} \sum_r C_{0,r} e^{-ikr} . \]
so that MI phase. The density in the ICP can be calculated from phase (ICP). For \( J > J_0^{\ast} \) there is no MI.

\( \frac{N}{r} \) is the number of sites of the 1D lattice.

The local density \( n_r \) and the correlation of the density fluctuations can be directly measured in an experiment. This motivates the following study of these quantities for a translational-invariant system as well as for a system with a weak parabolic potential. We wil compare the results in the incommensurate regime near the transition to the Mott insulator and discuss their characteristic properties.

(i) Translational-invariant case. For constant fugacity \( \zeta = \zeta_0 \) the system has translational symmetry on the sublattices, and \( G_{r,r'} \) can be calculated analytically.

Figure 1 shows the zero-temperature phase diagram of the model. The particle density is constant in space. Three phases can be identified: an empty phase with \( n = 0 \) for \( \zeta < 1/(1 + 2J) \), a Mott insulator (MI) with \( n = 1 \) for \( \zeta > 1/(1 + 2J) \) and \( J < 1/2 \), and an incommensurate phase (ICP). For \( J > J_0 = 1/2 \) the system exhibits no MI phase. The density in the ICP can be calculated from Eq. 4 and gives

\[
n = 1 - \frac{1}{2\pi} \left[ \tilde{k} + (k^\ast - \pi) \right], \tag{7}
\]

where \( \tilde{k} \) correspond to the cases \( \zeta > 1 \) and \( \zeta < 1 \), respectively, and \( \tilde{k} \), \( k^\ast \) are given by

\[
\tilde{k} = \arccos \left( 1 - \frac{(1 + \zeta^{-1})^2}{2(\zeta^{-1} + J^2)} \right), \tag{8}
\]

\[
k^\ast = \arccos \left( \frac{(1 - \zeta^{-1})^2}{2J^2} - 1 \right). \tag{9}
\]

The transition from the intermediate to the Mott insulating phase at the critical fugacity \( \zeta_c = 1/(1 - 2J) \) is continuous.

To investigate the behavior of the system near the Mott transition we calculate the correlations of density fluctuations asymptotically from Eq. 5 as

\[
C_{0,r} \sim \left( \frac{\sin (k^\ast r)}{\zeta r} \right)^2. \tag{10}
\]

After a Fourier transformation we obtain the static structure factor as

\[
S_k \sim \left\{ \begin{array}{ll}
\frac{\pi}{2k^\ast} (k^\ast - \frac{\pi}{2}) & : 0 < k < 2k^\ast \\
\frac{\pi}{2k^\ast} (k^\ast + \frac{\pi}{2}) & : 0 > -k > -2k^\ast \\
0 & : |k| > 2k^\ast
\end{array} \right. \tag{11}
\]

These quantities are shown in Fig. 2 a,b for two values of the tunneling rate \( J \) in the ICP. They vanish as the MI phase is reached due to the fact that the MI exhibits no density fluctuations. The correlation function of the density fluctuations shows significant oscillations in the ICP. Their wavelength \( \lambda = 2\pi/k^\ast \) determines the characteristic length scale for density fluctuations and diverges as the Mott transition is approached. \( S_k \) is nonzero in the interval \([-2k^\ast, 2k^\ast]\) and falls off linearly to both sides from \( k = 0 \). The slope of the static structure factor does not depend on the tunneling rate.

The dependence of \( k^\ast \) on the density for varying tunneling rates is depicted in Fig. 3. At low densities \( k^\ast \) increases with increasing \( n \) until it reaches its maximal value of \( \pi \) at a certain density, where it shows a cusp for \( J < \infty \). For \( J \leq J_0 \) the system can undergo a Mott transition, where \( k^\ast \) vanishes at \( n = 1 \). Otherwise it stays nonzero.

Note that these features of hard-core bosons in 1D differ fundamentally from those of an ideal Bose gas in 1D. There \( C_{0,r} \) decays exponentially and its oscillations show no characteristic behavior.

(ii) Parabolic background potential. A parabolic potential can be expressed as a spatially varying fugacity \( \zeta\prime = \zeta^{-1} + \Omega r^2 \), where \( \Omega \) determines the strength of the potential. In this case \( G_{r,r'} \) cannot be evaluated simply by a Fourier transformation, since the translational invariance is broken. We have calculated the local particle density, the correlations of the density fluctuations and the static structure factor by inverting the matrix \( \mathbf{R} \) numerically on a lattice with \( N = 500 \) sites.
The local particle density $n_r$ is shown in Fig. 4 for different values of the tunneling rate $J$. The density is symmetric around the minimum of the parabolic potential at $r = 0$ with a maximum at the center. It is suppressed as the potential becomes larger with increasing distance from the center of the trap. As the tunneling rate is decreased the distribution of the particles along the lattice becomes narrower and the density is shifted upwards. When $J$ reaches some value $J_P$, we observe a region with local particle density $n_r = 1$ developing symmetrically around $r = 0$.

To investigate the development of this plateau we have evaluated the correlations of the density fluctuations $C_{0,r}$ together with the associated static structure factor. These quantities are depicted in Fig. 2c,d for two
values of $J \gtrsim J_P$. The correlation function of the density fluctuations exhibits oscillations that do not have a unique wavelength and $S_k$ does not show a sharp cut-off. However, the properties are qualitatively the same as in the translational-invariant case. Both quantities vanish when $J_P$ is reached, owing to the fact that there are no density fluctuations within the plateau. The characteristic length scales become larger as the Mott plateau is approached. Close to $J_P$ we observe clear indications for the developing Mott plateau [17]. The correlations of the density fluctuations are suppressed around the center of the trap leading to a local minimum of $C_{0,r}$ at $r = 0$. This is accompanied by a decrease of the slope of $S_k$.

**Conclusion.** For the 1D strongly interacting Bose gas in an optical lattice we have identified characteristic oscillations of the density-density correlation function with length $\lambda$. This can be used as a measure for the distance of the system from the MI state: the length $\lambda$ diverges in units of the lattice spacing with the density $n$ as $1/(1-n)$ when we approach the MI. This phenomenon is related to the behavior of the static structure factor $S_k$ with characteristic wavevector $k^* = 2\pi/\lambda$. $S_k$ is linear and vanishes for $|k| > k^*$. $k^*$ itself vanishes continuously as the MI is approached and $S_k = 0$ in the MI phase. This behavior also survives qualitatively if a weak parabolic potential is applied to the interacting Bose gas. In particular, the static structure factor is strongly suppressed if a large fraction of the Bose gas is in the MI state.

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