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Cenap Ates, Christopher Moseley, Klaus G. Ziegler

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Density fluctuations of a hard-core Bose gas in a one-dimensional lattice near the Mott insulating phase

C. Ates, Ch. Moseley, and K. Ziegler*

Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany

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The characteristic oscillations of the density-density correlation function and the resulting structure factor are studied for a hard-core Bose gas in a one-dimensional lattice. Their wavelength diverges as the system undergoes a continuous transition from an incommensurate to a Mott insulating phase. The transition is associated with a unit static structure factor and a vanishing sound velocity. 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 in an optical lattice [1–3] have opened an exciting 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 (2D and 3D) systems but also prevent us from using conventional mean-field methods.

Strong repulsion allows at most one boson per minimum of the optical lattice. This situation has been realized in recent experiments [3]. In such a system there is a competition between repulsive and kinetic energy: For a sufficiently weak tunneling rate the repulsive energy always wins and a Mott insulator is formed. In the case of weak repulsion Mott insulators can also be formed at commensurable fillings of the optical lattice with $n=1,2,\ldots$ bosons at each potential minimum. Subsequently we shall only consider the case of strong repulsion.

A well-known fact of one-dimensional many-body physics is that a continuous hard-core Bose gas can be mapped to a free Fermi gas [4,5]. This can be understood when we study a grand-canonical ensemble of bosons. The bosons diffuse along the 1D lattice by tunneling between nearest-neighbor sites like free particles. They experience each other only when they try to tunnel to the same site at the same time. However, this process is excluded by the strong repulsion between the bosons. The exclusion condition is also an intrinsic statistical property of fermions as a consequence of the antisymmetry of the fermionic wave function under particle exchange. The fact that bosons have a symmetric wave function under particle exchange is irrelevant in 1D because particles cannot exchange their positions in this case. Therefore, free fermions and hard-core bosons are equivalent in 1D but not in higher dimensions.

For free fermions the multiparticle wave function (Slater determinant) factorizes in the diagonal representation of the individual particles. The partition function of a grand-canonical ensemble of fermions with Hamiltonian H at temperature $1/\beta$ then reads

$$Z = \mathrm{Tr} e^{-\beta H} = \prod_{\omega,k} z(\omega,k),$$

where ω is the Matsubara frequency and k is the wave vector for a translational-invariant 1D system. In order to determine $z(\omega,k)$ we will adopt an approach to the statistics of directed polymers [6] in two dimensions. The analogy with this classical statistical problem is based on the observation that the world lines of a grand-canonical ensemble of bosons are equivalent to directed polymers, random walks, or fluctuating flux lines [7,8]. This can be formally expressed by the fact that the partition function Z of the grand-canonical ensemble of these systems is identical.

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

$$Z = \prod_{\omega} \det \mathbf{R}(\omega), \tag{1}$$

where $\mathbf{R}$ is diagonal with respect to the Matsubara frequency ω,

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

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

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

$z(\omega,k)$ is obtained from $\mathbf{R}(\omega)$ by diagonalization with respect to the 1D lattice and the 2×2 structure.

This model describes the tunneling of bosons with rate $J \geqslant 0$ between nearest neighbors, expressed by the shift operator $\hat{T}$ and its inverse $\hat{T}^{-1}$. J is dimensionless and measured in units of the energy $\hbar^2/2ma^2$, where m is the mass of the particles and a the lattice constant. The 2×2 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

*Electronic address: klaus.ziegler@physik.uni-augsburg.de

second site, where ar is the position on a sublattice, and r takes integer values.

$\zeta > 0$ is the fugacity that controls the density of bosons in the system. Here, it is related to the chemical potential μ, which is measured in the same energy unit as J, by $\zeta^{-1} = 1 - \mu$. 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 ζ_r.

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

$$G_{r,r'} = \int_0^{2\pi} (\mathbf{R}^{-1})_{r,r'} \frac{d\omega}{2\pi} \tag{3}$$

to evaluate the local density of bosons as

$$n_r = 1 + \zeta_r^{-1} G_{r,r}. \tag{4}$$

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 [3–5,9–14] 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 $G_{r,r'}$ [6].

Another interesting quantity is the correlation function of the density fluctuations

$$C_{r,r'} = (\zeta_r \zeta_{r'})^{-1} G_{r,r'} G_{r',r} + \zeta_r^{-1} G_{r,r} \delta_{r,r'} \tag{5}$$

from which the static structure factor as a function of the momentum k can be obtained by Fourier transformation [15]

$$S_k := 1 - \sum_r (C_{0,r} + n_0 \delta_{r,0}) e^{-ikr} \Big/ \sum_r (C_{0,r} + n_0 \delta_{r,0}). \tag{6}$$

k is dimensionless and measured in units of $\hbar / a$.

The local density n_r and the correlation of the density fluctuations can be directly measured in an experiment [16]. 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 will 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 $\zeta_r \equiv \zeta$ the system has translational symmetry on the sublattices, and $G_{r,r'}$ can be calculated analytically [6]. 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

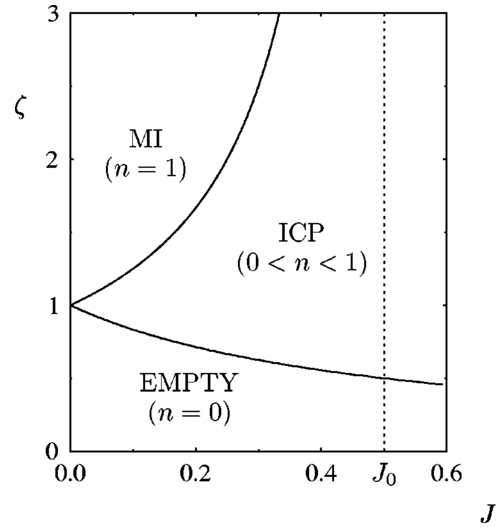

FIG. 1. The zero-temperature phase diagram of the model shows three phases: a Mott insulator (MI), an incommensurate (ICP), and an empty phase. For $J > J_0 = 1/2$ there is no MI.

$$n = 1 - \frac{1}{2\pi} [\tilde{k} \mp (k^\star - \pi)], \tag{7}$$

where $\mp$ correspond to the cases $\zeta > 1$ and $\zeta < 1$, respectively, and $\tilde{k}$, $k^\star$ are given by

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

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

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) for $r \gg 1$ and $k^\star \ll 1$ as

$$C_{0,r} \sim (\sin(k^\star r)/\zeta r)^2. \tag{10}$$

After a Fourier transformation we obtain the static structure factor as

$$S_k \sim \begin{cases} \dfrac{|k|}{2k^\star} & : \quad |k| < 2k^\star \\ 1 & : \quad |k| > 2k^\star \end{cases}. \tag{11}$$

These quantities are shown in Figs. 2(a) and 2(b) for two values of the tunneling rate J in the ICP. $C_{0,r}$ vanishes 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 $\lambda = 2\pi / k^\star$ determines the characteristic length scale for density fluctuations and diverges as the Mott transition is approached. S_k grows linearly to both sides from $k=0$ in the interval $[-2k^\star, 2k^\star]$ and is constantly 1 elsewhere. The Feynman relation $S_k = k^2 / 2m\hbar\omega(k)$ with the dispersion relation $\omega(k) = \hbar ck + \mathcal{O}(k^2)$, which is linear for small values

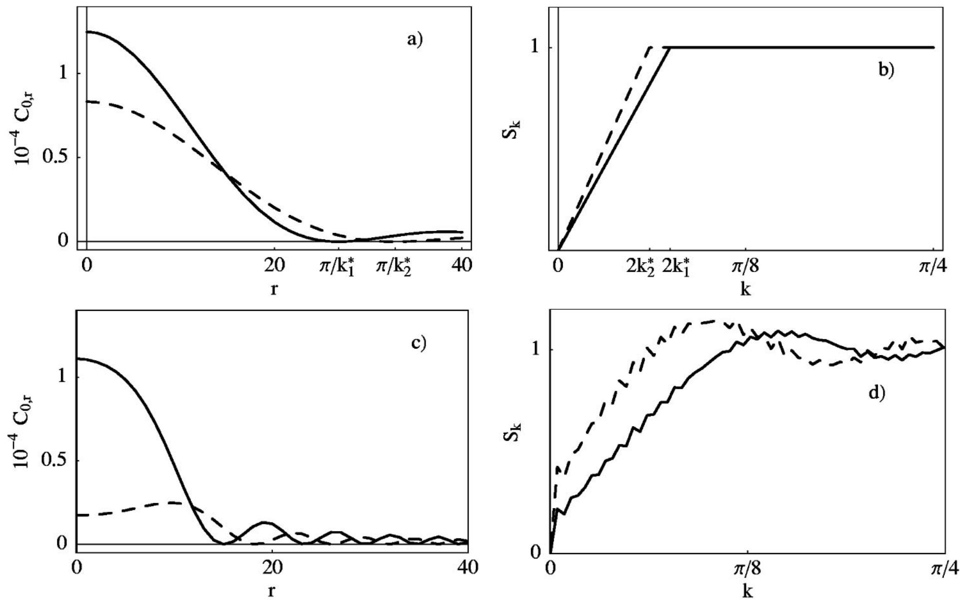

FIG. 2. Correlation function of density fluctuations $C_{0,r}$ and static structure factor S_k for different tunneling rates J. First row: constant background ($\zeta^{-1}=0.3$, $\Omega=0$). Second row: parabolic background ($\zeta^{-1}=0.3$, $\Omega=3\times10^{-5}$). Tunneling rates: $J_1=0.3506$ (solid lines) and $J_2=0.3504$ (dashed lines). The transition point for the Mott insulator is at $J=0.3500$.

of k, allows us to identify the sound velociy as $c=k^\star/m\hbar$.

The dependence of $k^\star$ on the density for varying tunneling rates is depicted in Fig. 3. At low densities $k^\star$ increases with increasing n until it reaches its maximal value of π at a certain density, where it shows a cusp for $J<\infty$. For $J\leqslant J_0$ the system can undergo a Mott transition, where $k^\star$ vanishes at $n=1$. Otherwise it is nonzero. This behavior is substantially different from the behavior of the continuous (Tonks-Girardeau) gas [4,15]. In the latter the role of $k^\star$ is played by k_F ($\equiv\pi n$) which depends linearly on the density. This difference reflects the fact that the lattice system undergoes a transition to a Mott insulating phase, in contrast to the continuous Bose gas which cannot become a Mott insulator without an additional potential. Recent experiments [1–3] were performed in a strong optical potential that can be described by a lattice model.

(ii) Parabolic background potential. A parabolic potential can be expressed as a spatially varying fugacity $\zeta_r^{-1}=\zeta^{-1}+\Omega r^2$, where Ω 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 [17]. 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 Figs. 2(c) and 2(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 cutoff. However, the properties are qualitatively the same as in the translational-invariant case. $C_{0,r}$ vanishes when J_P is reached, owing to the fact that there are no density fluctuations within the plateau. The char-

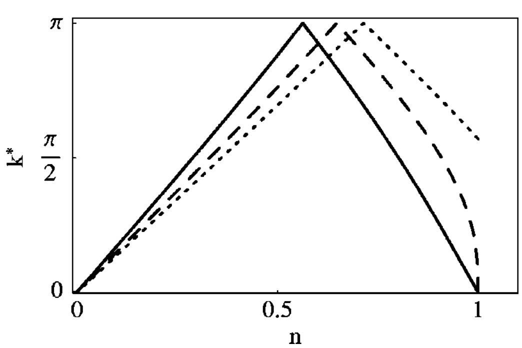

FIG. 3. Characteristic wave vector $k^\star$ as a function of the density in the translational-invariant case. Curves are plotted for different values of the tunneling rate: $J=0.2<J_0$ (solid), $J=0.5=J_0$ (dashed), $J=0.8>J_0$ (dotted).

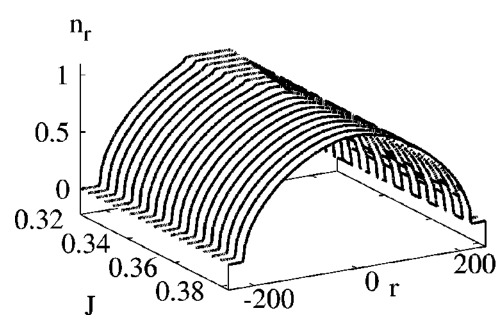

FIG. 4. Local particle density for parabolic background potential ($\zeta^{-1}=0.3$, $\Omega=3\times10^{-5}$). Development of a Mott plateau in the center of the trap ($r=0$) as the tunneling rate J is decreased below $J_P\approx0.35$.

acteristic length scales become larger as the Mott plateau is approached. Close to J_P we observe clear indications for the developing Mott plateau [18]. 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 an increase 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 λ. This can be used as a measure for the distance of the system from the MI state: the length λ 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. Its characteristic wave vector $k^{\star}=2\pi/\lambda$ is proportional to the sound velocity c. S_k is linear and saturates at a value of 1 for $|k|>2k^{\star}$. $k^{\star}$ itself vanishes continuously as the MI is approached and $S_k=1$ 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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