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# Interacting bosons in an optical lattice: Bose-Einstein condensates and Mott insulator

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A dense Bose gas with hard-core interaction is considered in an optical lattice. We study the phase diagram in terms of a special mean-field theory that describes a Bose-Einstein condensate and a Mott insulator with a single particle per lattice site for zero as well as for nonzero temperatures. We calculate the densities, the excitation spectrum, and the static structure factor for each of these phases.

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## I. INTRODUCTION

Optical lattices have opened an exciting field of physics. We are expecting new phenomena in comparison with continuous systems due to the lack of Galilean invariance. Among the most obvious consequences of the lattice structure is the formation of lattice-commensurate ground states like the Mott insulating phase. The latter was observed in experiments [1,2].

Light scattering on a Bose gas is strongly affected by the nature of the quasiparticles [3,4]. This provides a useful experimental tool to distinguish between different phases of the Bose gas. We expect, for instance, that light scattering by the gapless quasiparticle spectrum of the Bose-Einstein condensate (BEC) is quite different from light scattering in the gapful quasiparticle spectrum of the Mott insulator (MI). A physical quantity that is directly related to light scattering is the structure factor [4–9] which was measured in the case of a BEC [3]. This is also of interest in the Mott insulating phase [10,11]. In this paper we will study the static structure factor. Of particular interest is its behavior near the transition from the BEC to the MI. We will also study the phases and phase transitions for zero temperature as well as for nonzero temperature. For this purpose we will consider here a hard-core Bose gas in an optical lattice. Our model can be understood as a projection of the more general Bose-Hubbard model in the vicinity of those points of the phase diagram, where two adjacent Mott lobes meet (Fig. 1). This is similar to the picture which was applied to the tips of the Mott lobes in a recent paper by Huber *et al.* [8]. It is based on the following idea. The number of bosons per site is fixed in the Mott state. For adjacent Mott lobes this means that the corresponding Mott states differ exactly by one boson per site. Now we consider two adjacent lobes with  $n$  and  $n+1$  ( $n \geq 0$  bosons per site), respectively, and assume that the chemical potential is fixed such that the ground state is the Mott state with  $n$  particles per site. Low-energy excitations of this state for a grand-canonical system are states where one or a few sites (let us say  $k \geq 1$  sites) have  $n+1$  bosons, all other sites have  $n$  bosons. The  $k$  excessive bosons are relatively free to move from site to site on top of the  $n$  Mott state. Therefore the physics of these excitations can be described approximately by the tunneling of the  $k$  excessive bosons alone. Due to the repulsion of order  $U$ , assumed to be not too small, it is unlikely that a site with  $n+2$  bosons is created. Consequently, these excessive bosons form a hard-core Bose gas.

A hard-core boson can be represented by a pair of locally coupled spin-1/2 fermions. Here we will use the model introduced to study the dissociation of bosonic molecules into pairs of spin-1/2 fermionic atoms [12]. A functional integral with a two-component complex field was derived for this model that allowed a mean-field approximation. The latter revealed a zero-temperature phase diagram for a grand-canonical ensemble of bosons with three phases: an empty phase, a BEC, and a MI. This result is remarkable since previous mean-field calculations, using the same type of fermionic model as the starting point (e.g., using an  $N \rightarrow \infty$  limit [13]) did not give the entire phase diagram by ignoring the MI phase. Apparently, the form of the phase diagram depends crucially on the type of Hubbard-Stratonovich transformation that replaces the fermionic (i.e., Grassmann) fields by bosonic (i.e., complex) fields.

The structure of this paper is as follows. In Sec. II we discuss briefly the model and some related physical quantities. A mean-field approximation is used in Sec. III, where we derive the phase diagram. Gaussian fluctuations around the mean-field solution and its consequences are considered in Sec. IV. In this section we calculate the static structure factor, and in Sec. V we discuss our results. Details of our calculations are given in Appendixes A and B.

## II. THE MODEL

A hard-core Bose gas is considered on a  $d$ -dimensional hypercubic lattice with  $\mathcal{N}$  sites. Bosons can tunnel between these sites from a lattice site  $r$  to any of the nearest-neighbor

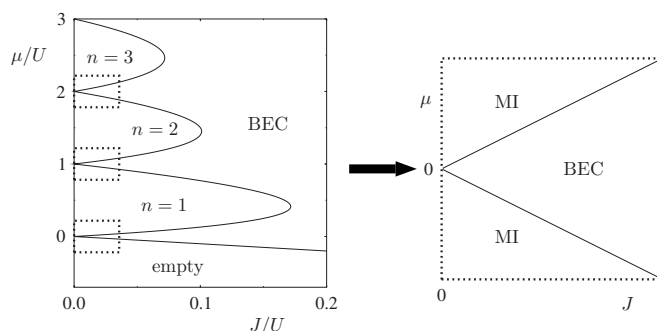


FIG. 1. A projection of the phase diagram of the Bose-Hubbard model in the vicinity of the point, where the two Mott lobes meet.  $\mu$  and  $J$  are in arbitrary energy units after the projection.

sites  $r'$ . Each boson consists of two fermions. Single fermions in this model cannot exist (i.e., in contrast to the model studied in Ref. [12] we do not allow dissociation of the bosonic molecules.) The Hamiltonian of the  $d$ -dimensional system is

$$\hat{H} = -\frac{J}{2d} \sum_{\langle r, r' \rangle} c_{r\uparrow}^\dagger c_{r'\uparrow}^\dagger c_{r'\downarrow}^\dagger c_{r\downarrow}^\dagger - \mu \sum_r \sum_{\sigma=\uparrow, \downarrow} c_{r\sigma}^\dagger c_{r\sigma}, \quad (1)$$

where the sum in the first term on the right-hand side is restricted to nearest neighbors, and  $c_{r\sigma}^\dagger$  and  $c_{r\sigma}$  are the creation and annihilation operators of the fermion with spin  $\sigma$  at site  $r$ , respectively. The first term describes tunneling of local fermion pairs in the optical lattice between nearest-neighbor sites with rate  $J$ . The chemical potential  $\mu$  controls the number of particles in a grand-canonical ensemble. The latter is given by the partition function

$$Z = \text{Tr} e^{-\beta \hat{H}}. \quad (2)$$

The partition function can also be written in terms of a Grassmann integral [14] as

$$Z = \int e^{-A(\psi, \bar{\psi})} D[\psi, \bar{\psi}] \quad (3)$$

with imaginary time-dependent conjugated Grassmann fields  $\psi$ ,  $\bar{\psi}$  and the action

$$A = \int_0^\beta dt \left[ \sum_r (\psi_r^1 \partial_t \bar{\psi}_r^1 + \psi_r^2 \partial_t \bar{\psi}_r^2) - \mu \sum_r (\psi_r^1 \bar{\psi}_r^1 + \psi_r^2 \bar{\psi}_r^2) - \frac{J}{2d} \sum_{\langle r, r' \rangle} \psi_r^1 \bar{\psi}_{r'}^1 \psi_r^2 \bar{\psi}_{r'}^2 \right]. \quad (4)$$

Applying the concept of linear response to the quasiparticles, we obtain the dynamic structure factor with the definition [5]

$$S(q, \omega) = \sum_{n, m} e^{-\beta \hbar \omega_m} |\langle n | \hat{\rho}_q^\dagger - \langle \hat{\rho}_q^\dagger | m \rangle|^2 \delta(\hbar \omega - \hbar \omega_{n, m}), \quad (5)$$

where  $\rho_q^\dagger$  is the Fourier transform of the atomic density operator at wave vector  $q$  and  $\omega_{n, m}$  is the frequency difference between energy level  $m$  and  $n$ . We treat an excited state  $n$  as one of the quasiparticles energy levels with  $\hbar \omega_{n, 0} = \epsilon_n$  within our approximation. Then the static structure factor is defined as [5]

$$S(q) = \frac{\hbar}{N} \int S(q, \omega) d\omega = \frac{1}{N} (\langle \rho_q \rho_{-q} \rangle - |\langle \rho_q \rangle|^2). \quad (6)$$

For small but nonzero  $T$ , when quasiparticles can be treated as noninteracting within the accuracy of the Bogoliubov approach for the weakly interacting Bose gas modified for an optical lattice we get [5]

$$S(q) = \frac{J g_q}{\epsilon_q} \coth \frac{\beta \epsilon_q}{2}, \quad (7)$$

where

$$g_q = 1 - \frac{1}{d} \sum_{i=1}^d \cos q_i. \quad (8)$$

For  $T=0$

$$S(q) = \frac{J g_q}{\epsilon_q}, \quad (9)$$

where  $\epsilon_q$  is the quasiparticle spectrum.

This result was obtained within the mean-field approximation to the weakly interacting Bose gas. It is interesting to compare this result with the result obtained by a direct calculation for our model within our mean-field approach. Using Eq. (6) the static structure factor can be calculated as [15]

$$S(q) = \frac{1}{N} \sum_{r, r'} C_{r, r'} e^{iq(r-r')}, \quad (10)$$

where the truncated density-density correlation function is

$$C_{r, r'} = \langle n_r n_{r'} \rangle - \langle n_r \rangle \langle n_{r'} \rangle. \quad (11)$$

Introducing spatial coordinates  $p = \{r, t\}$  the static structure factor reads

$$S(q) \equiv \frac{1}{\beta N} \sum_{r, r'} \int_0^\beta dt \int_0^\beta dt' C_{rt, r't'} e^{iq(r-r')}. \quad (12)$$

This expression will be studied within mean-field theory and Gaussian fluctuations.

### III. MEAN-FIELD APPROXIMATION: PHASE DIAGRAM

The mean-field approximation cannot be directly applied to the Grassmann fields. Therefore, we perform a Hubbard-Stratonovich transformation in order to replace the Grassmann fields by complex fields. This leads to an effective action depending on complex fields. As we already mentioned in the Introduction, the form of the Hubbard-Stratonovich transformation is not unique. Here we use the version given in Ref. [12] because it provides the proper phase diagram. First of all we decouple the fourth order term in the action using the identity

$$\begin{aligned} & \exp \left( \frac{J}{2d} \sum_{\langle r, r' \rangle} \psi_r^1 \bar{\psi}_{r'}^1 \psi_r^2 \bar{\psi}_{r'}^2 \right) \\ &= \int [d\phi][d\chi] \exp \left( - \sum_{r, r'} \bar{\phi}_r \hat{v}_{r, r'}^{-1} \phi_{r'} - \frac{1}{2J} \sum_r \bar{\chi}_r \chi_r \right. \\ & \quad \left. - \sum_r (i\phi_r + \chi_r) \psi_{r,1} \psi_{r,2} - \sum_r (i\bar{\phi}_r + \bar{\chi}_r) \bar{\psi}_{r,1} \bar{\psi}_{r,2} \right). \end{aligned} \quad (13)$$

Summation over  $t$  in the last formula is implicitly assumed. In this formula the expression

$$\hat{v}_{r, r'} = J \left( \frac{1}{2d} \delta_{|r-r'|, 1} + 2\delta_{r, r'} \right) \quad (14)$$

was introduced. Moreover, the introduction of the auxiliary field  $\chi$  makes the matrix  $\hat{v}$  positive definite.

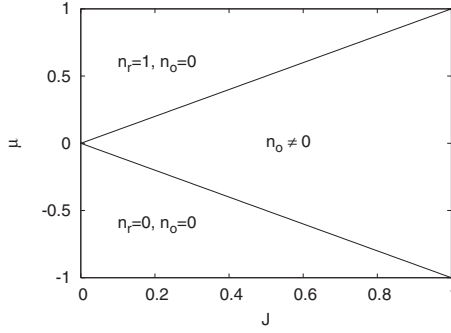


FIG. 2. Phase diagram for  $k_B T=0$ .  $\mu$  and  $J$  are in arbitrary energy units.

A subsequent integration over Grassmann fields leads to

$$A_{\text{eff}} = \int_0^\beta dt \left\{ \sum_{r,r'} \bar{\phi}_r \hat{v}_{r,r'}^{-1} \phi_{r'} + \frac{1}{2J} \sum_r \bar{\chi}_r \chi_r - \ln \det \hat{\mathbf{G}}^{-1} \right\} \quad (15)$$

with

$$\hat{\mathbf{G}}^{-1} = \begin{pmatrix} -i\phi - \chi & \partial_\tau + \mu \\ \partial_\tau - \mu & i\bar{\phi} + \bar{\chi} \end{pmatrix}, \quad \hat{v} = J(\hat{\omega} + 2\hat{1}),$$

$$\hat{\omega}_{r,r'} = \begin{cases} 1/2d, & r, r' - \text{nearest neighbors} \\ 0, & \text{otherwise.} \end{cases}$$

The partition function now reads

$$Z = \int e^{-A_{\text{eff}}(\phi, \chi)} D[\phi, \chi]. \quad (16)$$

In the following, we make the replacement  $\mu \rightarrow \mu/2$ , such that  $\mu$  plays the role of the chemical potential of the molecules. We can perform a saddle-point integration to calculate physical quantities. From a physical point of view we have to minimize our action to get the classical trajectory (i.e., the macroscopic wave function) of our system. Fluctuations around this trajectory are caused by thermal and quantum effects. The mean-field solution characterizes the condensed phase, in which  $|\phi|$  has a nonzero value. Fluctuations describe quasiparticle excitations above the condensate. In order to proceed within a mean-field approximation we assume that quantum fluctuations are small.

Minimization of the action gives us two coupled linear equations between the complex fields  $\phi$  and  $\chi$ :

$$\delta A_{\text{eff}} = 0 \Rightarrow \begin{cases} \phi = 3JG(\phi - i\chi), \\ \chi = -i2JG(\phi - i\chi), \end{cases} \quad (17)$$

where

$$G = \frac{1}{\beta} \sum_{\omega_n} \frac{1}{|\phi|^2/9 + \mu^2/4 + \omega_n^2}.$$

A solution of these equations is

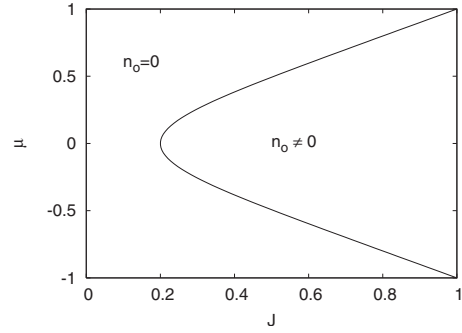


FIG. 3. Phase diagram for  $k_B T=0.05J$ .  $\mu$  and  $J$  are in arbitrary energy units.

$$G = \frac{1}{J}, \quad \chi = -\frac{2i\phi}{3}. \quad (18)$$

In these equations  $\omega_n = (2n+1)\pi/\beta$  are the Matsubara frequencies of the fermions. This leads to (we perform the rescaling  $4|\phi|^2/9 \rightarrow |\phi|^2$ )

$$J = \sqrt{\mu^2 + |\phi|^2} \left( \frac{e^{\beta\sqrt{\mu^2 + |\phi|^2}/2} + 1}{e^{\beta\sqrt{\mu^2 + |\phi|^2}/2} - 1} \right) \quad (19)$$

and within the saddle-point integration we obtain the expression for the local density

$$n = \frac{1}{\beta\mathcal{N}} \frac{\partial \ln Z}{\partial \mu} = \frac{1}{2} + \frac{1}{2} \frac{\mu}{\sqrt{\mu^2 + |\phi|^2}} \left( \frac{e^{\beta\sqrt{\mu^2 + |\phi|^2}/2} - 1}{e^{\beta\sqrt{\mu^2 + |\phi|^2}/2} + 1} \right). \quad (20)$$

It should be noticed that this expression for  $J=0$  and  $T=0$  gives a correct result, which can alone be obtained by direct calculations. The corresponding phase diagram is depicted in Figs. 2 and 3 with the phase boundary given by  $\phi=0$ .

With the result given in Eq. (20) we can evaluate the local compressibility:

$$k_r = \left( \frac{\partial n_r}{\partial \mu} \right)_T. \quad (21)$$

For  $T=0$  and small  $|\phi|^2$  it reads

$$k_r \approx \frac{|\phi|^2}{2\mu^3}. \quad (22)$$

The local compressibility is not divergent within our mean-field approximation, which is typical in the case of optical lattices [16–18].

We see that this model gives three phases. It can describe both the dilute regime and the dense regime, as a consequence we have the empty phase along with the MI phase.

A few words about the type of phase transitions. Near the phase transition the order parameter is small, so that we may apply a perturbative expansion:

$$A_{\text{eff}} = \underbrace{\frac{1}{J} \frac{|\phi|^2}{9} - \frac{1}{\beta} \sum_{\omega_n} \frac{1}{\mu^2 + \omega_n^2} \frac{|\phi|^2}{9}}_{\text{can be negative}} + \underbrace{\frac{1}{2\beta} \sum_{\omega_n} \frac{1}{(\mu^2 + \omega_n^2)^2} \frac{|\phi|^4}{81}}_{>0} + O(|\phi|^6). \quad (23)$$

The first term can be negative, such that the order parameter may differ from zero. The order parameter vanishes continuously indicating that we have a second order phase transition.

#### IV. GAUSSIAN FLUCTUATIONS AROUND MEAN-FIELD SOLUTION

The complex fields  $\phi_x$  and  $\chi_x$  are expected to fluctuate about the SP solution due to thermal and quantum effects. Denote  $\Delta = i\phi + \chi$  and  $\bar{\Delta} = i\bar{\phi} + \bar{\chi}$ , then

$$\hat{\mathbf{G}}^{-1} = \hat{\mathbf{G}}_0^{-1} + \begin{pmatrix} -\delta\Delta & 0 \\ 0 & \delta\bar{\Delta} \end{pmatrix}, \quad (24)$$

where

$$\hat{\mathbf{G}}_0^{-1} = \begin{pmatrix} -\Delta_0 & \partial_\tau + \mu \\ \partial_\tau - \mu & \bar{\Delta}_0 \end{pmatrix}.$$

Applying the Taylor expansion  $\ln(1+x) = x - x^2/2 + \dots$  we get

$$\begin{aligned} \ln \det \hat{\mathbf{G}}^{-1} &= \text{tr} \ln \hat{\mathbf{G}}^{-1} \\ &= \text{tr} \ln \left[ \hat{\mathbf{G}}_0^{-1} + \begin{pmatrix} -\delta\Delta & 0 \\ 0 & \delta\bar{\Delta} \end{pmatrix} \right] \\ &\approx \text{tr} \ln \hat{\mathbf{G}}_0^{-1} - \frac{1}{2} \text{tr} \left[ \hat{\mathbf{G}}_0 \begin{pmatrix} -\delta\Delta & 0 \\ 0 & \delta\bar{\Delta} \end{pmatrix} \right]^2. \end{aligned} \quad (25)$$

Calculating the trace in the  $p=\{q, \omega\}$  representation we get

$$Z \sim \int D[\delta\phi] \exp[-\delta A_{\text{eff}}], \quad (26)$$

where  $\delta A_{\text{eff}}$  is given in Appendix A. This has the form of an inverse Green's function  $\hat{G}^{-1}$  with imaginary time for quasiparticles, which is described by fields  $\delta\phi$ . By applying the spectral representation of the Green's function we can identify the poles of function  $\hat{G}$ , namely  $i\omega$  with the excitation spectrum of the quasiparticles. The exact solution in the condensed phase is

$$\epsilon_q = \sqrt{g_q(J^2 - \mu^2) + g_q^2 \mu^2}. \quad (27)$$

In the dilute regime, where  $\mu+J$  is small, and for small  $q$  we get the Bogolubov spectrum with an effective mass of the bosons  $\sim 1/J$  and sound velocity  $\approx \sqrt{2J\tilde{\mu}}$  (we used  $\tilde{\mu}=J+\mu$ ). This has the same form as the quasiparticle spectrum obtained in [13].

In the empty phase and in the MI phase we have excitations with a gap:

$$\epsilon_q = |\mu| - J + Jg_q. \quad (28)$$

The symmetric form of the results for the MI phase and for the empty phase is due to the particle-hole symmetry of our model.

In the dilute regime (small  $\tilde{\mu}=J+\mu$ ) and for low temperatures, including fluctuations, we obtain

$$n_0 = n - \sum_{q \neq 0} n_q \approx \tilde{\mu} \int \frac{dq}{Jg_q} - (k_B T)^{3/2} \int \frac{d^3 q}{(2\pi)^3} \frac{1}{e^{g_q} - 1}. \quad (29)$$

This result is in good agreement with a weakly interacting Bose gas with an effective chemical potential  $\tilde{\mu}$  [19].

#### A. Quantum fluctuations versus thermal fluctuations

By defining the condensed density in the following way,

$$n_o = \lim_{|r-r'| \rightarrow \infty} \langle c_{r\uparrow}^\dagger c_{r'\uparrow} c_{r\downarrow}^\dagger c_{r'\downarrow} \rangle = \lim_{|r-r'| \rightarrow \infty} \langle \psi_r^1 \bar{\psi}_{r'}^1 \psi_r^2 \bar{\psi}_{r'}^2 \rangle,$$

we arrive at the expression for the condensed density, which can be calculated as

$$\lim_{|r-r'| \rightarrow \infty} \int_0^\beta dt \int_0^\beta dt' \times \left\langle \frac{-\Delta_{rt} \bar{\Delta}_{r't'}}{(-\partial_t^2 + \mu^2/4 - \Delta_{rt} \bar{\Delta}_{rt})(-\partial_{t'}^2 + \mu^2/4 - \Delta_{r't'} \bar{\Delta}_{r't'})} \right\rangle.$$

Then fluctuating fields  $\Delta = \Delta_0 + \delta\Delta$ , expanding the above expression up to the second order of  $\delta\Delta$ , and using the Green's function given in Appendix A, we arrive at

$$n_o = \frac{(J^2 - \mu^2)}{4J^2} + \delta n_o, \quad (30)$$

where the correction due to the quantum fluctuations to the mean-field result is

$$\begin{aligned} \delta n_o &= -\frac{(J^2 - \mu^2)\mu^2}{J^3} \int \frac{d^d k}{(2\pi)^d} \frac{B_k^2 g_k}{\epsilon_k} + \frac{(J^2 - \mu^2)}{4J^3} \int \frac{d^d k}{(2\pi)^d} B_k \epsilon_k \\ &\quad - \frac{(J^2 - \mu^2)^2}{4J^3} \int \frac{d^d k}{(2\pi)^d} \frac{B_k^2}{\epsilon_k} \\ &\quad + \frac{3(J^2 - \mu^2)^2 \mu^2}{4J^5} \int \frac{d^d k}{(2\pi)^d} \frac{B_k^2 g_k}{\epsilon_k}. \end{aligned}$$

The main correction due to the thermal fluctuations are already included in our mean-field theory, where the condensed density is given by

$$n_o = \frac{|\phi|^2/4}{J^2}, \quad (31)$$

and  $|\phi|^2$  can be determined from Eq. (19).

The effect of quantum fluctuations and thermal fluctuations is depicted in Fig. 4. We see that both of them lead to a depletion of the condensate, but the quantum depletion alone does not change the transition points.

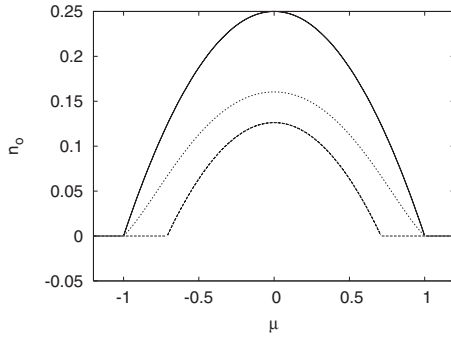


FIG. 4. Condensed density. The solid, dotted, and dashed lines show the mean-field result at  $k_B T = 0$ , the influence of the quantum fluctuations at  $k_B T = 0$  to the mean-field result and the mean-field result at  $k_B T = 0.2J$ , respectively.  $\mu$  and  $J$  are in arbitrary energy units.

### B. Static structure factor

The static structure factor is a Fourier transform of the truncated density-density correlation function. The latter contains the nonlocal term

$$\begin{aligned} & \langle \psi_r^1 \psi_r^2 \bar{\psi}_r^1 \bar{\psi}_r^2 \psi_{r'}^1 \psi_{r'}^2 \bar{\psi}_{r'}^1 \bar{\psi}_{r'}^2 \rangle \\ &= \int_0^\beta dt \int_0^\beta dt' \\ & \times \left\langle \frac{1}{(-\Delta_{rr} \bar{\Delta}_{rr} - \partial_t^2 + \mu^2/4)(-\Delta_{r'r'} \bar{\Delta}_{r'r'} - \partial_{t'}^2 + \mu^2/4)} \right\rangle. \end{aligned} \quad (32)$$

In mean-field approximation the truncated density-density correlation function should vanish [12]. Taking into account fluctuations, we write again  $\Delta = \Delta_0 + \delta\Delta$ ,  $\bar{\Delta} = \bar{\Delta}_0 + \delta\bar{\Delta}$  and substitute it into Eq. (32). Then expanding up to the second order and Fourier transforming the obtained expression, after a direct but lengthy calculation we get for small wave vectors  $q$  and for low temperatures  $T$  in the BEC phase

$$S(q) \sim \frac{(J^2 - \mu^2) J g_q}{J^2 n \epsilon_q} \coth \frac{\beta \epsilon_q}{2}, \quad (33)$$

where  $n$  is the total density of particles.

In the dilute regime, i.e., close to the empty phase, when  $n \sim (J + \mu)/J$  and  $J - \mu \approx 2J$  we obtain

$$S(q) \sim \frac{J g_q}{\epsilon_q} \coth \frac{\beta \epsilon_q}{2},$$

which is in agreement with the well-known result for the weakly interacting Bose gas [5]. In the dense regime, i.e., close to the Mott phase when  $n \approx 1$ , the static structure factor vanishes. The dependence of the static structure factor on  $q$  in the dilute regime is depicted in Fig. 5.

The static structure factor measures the density-density correlations in  $q$  space. Assuming that the thermal energy is much larger than the gap (i.e.,  $k_B T \gg \Delta$ ), the maximum of the structure factor appears at  $q$  values for which the following condition holds:

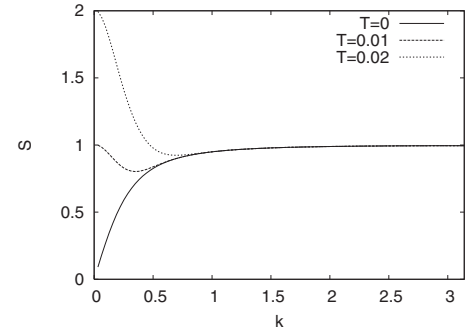


FIG. 5. Static structure factor in the BEC phase in the dilute regime,  $\mu = -0.99J$ .  $J$  is in arbitrary energy units. The unit of length is the lattice constant, so  $k$  is dimensionless.

$$J g_q \approx \Delta, \quad (34)$$

where  $\Delta = \mu - J$  is an energy gap in the excitation spectrum. Thus fluctuations begin to feel each other at the distance equal to their effective size  $r \sim 1/q \sim 1/\sqrt{\mu - J}$ .

Spatial correlations can be calculated by Fourier transforming the static structure factor. Near the phase transition for  $T=0$  we have in the condensed phase for large  $r$  (see Appendix B)

$$C_{r,0} = \sum_q S(q) e^{iqr} \sim \frac{1}{r^{d+1}}. \quad (35)$$

A similar behavior was found for a one-dimensional lattice in [7].

### V. DISCUSSION

A paired-fermion model for bosons with a hard-core interaction was studied. The effective Hamiltonian is given by Eq. (1). Both phases, the BEC and the MI phase, were found within the same mean-field approach to our model.

In the BEC phase there is a long-range order in the phase fluctuations (i.e., phase coherence) and quasiparticles have a linear excitation spectrum for small momenta  $q$ . This reflects the existence of a Goldstone mode due to the breaking of a global U(1) gauge symmetry. Approaching the MI phase the system loses its phase coherence at the transition point and the excitation spectrum is characterized by the gap opening.

In previous calculations, performed on the Bose-Hubbard model, each phase requires its own specific mean-field approach [20,21] or a single one close to the phase boundary [8]. In the MI phase our expression for the excitation spectrum agrees with the branch of the excitation spectrum, which corresponds to creation of holes in the first Mott lobe of the Bose-Hubbard model, taking the limit of a large interaction. However, the second branch, which corresponds to formation of doubly occupied sites, does not exist in our model since we can create only holes in the singly occupied lattice to excite our system and not additional particles due to the hard-core condition. This is possible in the grand-canonical ensemble, where only the average number is fixed but the number of particles fluctuates.



Within a Bogoliubov approximation to the Bose-Hubbard model the quasiparticle spectrum in the BEC phase was found as [20,21]

$$\epsilon_q = \sqrt{J^2 g_q^2 + 2Un_0 J g_q},$$

where  $U$  is the interaction parameter and  $n_0$  is the condensate density. In contrast to this expression, we found for the spectrum the expression in Eq. (27). These expressions do not agree in the limit  $U \rightarrow \infty$ . Thus our hard-core Bose gas cannot be described within the Bogoliubov approximation to the Bose-Hubbard model by simply sending  $U$  to infinity. On the other hand, our results are in good agreement with a variational Schwinger-boson mean-field approach to the Bose-Hubbard model, which describe the phases near the phase transition, by sending  $U$  to infinity [8].

By changing the particle density from low to high values we pass from the weakly to strongly interacting regime. Within our approximation we were able to calculate an effect of quantum and thermal fluctuations on the condensate. The thermal fluctuations have a strong effect: They destroy the phase boundaries in a direction of its vanishing. For fixed tunneling rate  $J$  and chemical potential  $\mu$  one can determine a critical temperature at which the condensate vanishes. The quantum fluctuations do not change phase boundaries.

### A. Critical exponents

Our expansion of the action  $A_{\text{eff}}$  near the phase transition between the BEC and the Mott insulator Eq. (23) is similar to the Ginzburg-Landau theory of (thermal) phase transitions if we use the relation

$$\frac{T - T_c}{T_c} \rightarrow \frac{\mu - J}{J} \quad (36)$$

and  $\mu_c = J$ , i.e., the chemical potential  $\mu$  plays the role of the temperature  $T$  in our zero-temperature phase diagram. Within our approximation we find the mean-field expressions for three critical exponents: The critical exponent of the correlation length  $\xi$  of density fluctuations is  $\nu = 1/2$ , of the compressibility  $\chi$  it is  $\gamma = 1$ , and of the order parameter  $\phi$  it is  $\beta = 1/2$ . These critical exponents characterize the divergence of the corresponding quantities at the phase transition:

$$\xi \sim (\mu - J)^{-\nu}, \quad \chi \sim (\mu - J)^{-\gamma}, \quad \phi \sim (\mu - J)^\beta.$$

### B. Static structure factor

One possibility to detect the phase transition between the BEC and the MI in an optical lattice is to probe the excitation spectrum [1,22]. In the superfluid phase a broad continuum of excitations is observed but in the MI phase a more structured spectrum is measured, indicating the existence of the gap. The static structure factor vanishes in the Mott phase, as can be detected in experiments when studying phase transitions in an optical lattice.

We also notice that the particle density cannot serve as an order parameter for the BEC-MI transition and the scaling law is not applicable for density-density correlations, which can be determined as a Fourier transform of the static struc-

ture factor and is given in Appendix B. However, we can assume the validity of the scaling law for correlations of the order parameter, namely

$$\langle \delta\phi_r^* \delta\phi_{r'} \rangle. \quad (37)$$

Knowing the Green's function (see Appendix A) we obtain the following expression:

$$\langle \delta\phi_p \delta\phi_{-p'} \rangle = \delta_{p,p'} G_p \sim \delta_{p,p'} \frac{1}{\epsilon_q}. \quad (38)$$

Then for large distances  $r$  and for  $J = \mu$  (i.e., at the phase transition) we find the power law

$$C_{0,r} \sim \int d^d r \langle \delta\phi_p \delta\phi_{-p} \rangle e^{iqr} \sim \int d^d q \frac{\text{const}}{q^2} e^{iqr} \sim \frac{1}{r^{d-2}}, \quad (39)$$

which gives the anomalous exponent  $\eta = 0$  as in a mean-field Landau-Ginzburg theory.

## VI. CONCLUSIONS

We have used a paired-fermion model to describe strongly interacting bosons in an optical lattice with hard-core interaction. On the level of a mean-field theory we calculate the phase diagram, which includes the BEC and the MI. Including Gaussian fluctuations, we have found that the dispersion of quasiparticles is gapless in the BEC phase but has a gap in the MI phase:

$$\epsilon_q^{\text{BEC}} = \sqrt{g_q(J^2 - \mu^2) + g_q^2 \mu^2},$$

$$\epsilon_q^{\text{MI}} = \mu - J + J g_q.$$

$g_q$  is the dispersion of the bosons on the lattice, defined in Eq. (8).

We have calculated the total density, the condensate density, and the static structure factor. We have shown that the quantum fluctuations as well as thermal fluctuations lead to a depletion of the condensate, but the former do not change the critical points. The static structure factor contains information about the quasiparticle excitations and in the BEC phase for small  $q$  it is

$$S(q) \sim \frac{(J^2 - \mu^2) J g_q}{J^2 \epsilon_q} \coth \frac{\beta \epsilon_q}{2}.$$

It vanishes in the MI phase. For the critical behavior of the compressibility, the density correlations, and the order parameter at the phase transition between the BEC and the MI phase we found typical mean-field results.

## APPENDIX A: GREEN'S FUNCTION

In this appendix we write out the expression for the Green's function in both cases  $|\phi| = 0$  and  $|\phi| \neq 0$ . We denote  $p = \{q, \omega\}$ .

### 1. Case: $|\phi| = 0$

Deviation of the effective action due to fluctuations is

$$\delta A_{\text{eff}} = \sum_p (\delta\phi_p, \delta\chi_p) \overbrace{\begin{pmatrix} v_p^{-1} - D(p) & iD(p) \\ iD(p) & \frac{1}{2J} + D(p) \end{pmatrix}}^{G^{-1}} \begin{pmatrix} \delta\bar{\phi}_p \\ \delta\bar{\chi}_p \end{pmatrix}, \quad (\text{A1})$$

where

$$D(p) = \frac{1}{|\mu| - i\omega}, \quad v_p^{-1} = \frac{1}{J(3 - g_q)}.$$

The determinant of the Green's function reads

$$G^{-1} = \begin{pmatrix} v_p^{-1} - D(p) & iD(p) & -a & ia \\ iD(p) & \frac{1}{2J} + D(p) & ia & a \\ -a & ia & v_p^{-1} - D(-p) & iD(-p) \\ ia & a & iD(-p) & \frac{1}{2J} + D(-p) \end{pmatrix}, \quad (\text{A4})$$

where

$$D(p) = \frac{1}{2} \frac{\mu^2 + J^2 + 2i\mu\omega}{J(J^2 + \omega^2)},$$

$$D(-p) = \frac{1}{2} \frac{\mu^2 + J^2 - 2i\mu\omega}{J(J^2 + \omega^2)},$$

$$a = -\frac{1}{2} \frac{|\Phi|^2/9}{J(J^2 + \omega^2)}.$$

The determinant of the Green's function is

$$\det G^{-1} = \frac{1}{[2J^2(3 - g_q)]^2(J^2 + \omega^2)} [\omega^2 + (J^2 - \mu^2)g_q + \mu^2 g_q^2]. \quad (\text{A5})$$

$$\det G^{-1} = \frac{v_p^{-1}}{2J} - D(p) \left( \frac{1}{2J} - v_p^{-1} \right). \quad (\text{A2})$$

## 2. Case: $|\phi| \neq 0$

Deviation of the effective action due to fluctuations is

$$\delta A_{\text{eff}} = \sum_{p>0} (\delta\phi_p, \delta\chi_p, \delta\bar{\phi}_{-p}, \delta\bar{\chi}_{-p}) G^{-1} \begin{pmatrix} \delta\bar{\phi}_p \\ \delta\bar{\chi}_p \\ \delta\phi_{-p} \\ \delta\chi_{-p} \end{pmatrix} \quad (\text{A3})$$

with the Green's function

## APPENDIX B: CORRELATIONS

The decay of the density-density correlation function can be investigated as the inverse Fourier transform of the static structure factor

$$C_{r,0} \sim \frac{(J^2 - \mu^2)}{J^2} \int d\vec{q} \frac{J g_q}{\epsilon_q} e^{i\vec{q} \cdot \vec{r}}.$$

For large values of  $r$  the main contribution to the integral is for small values of  $q$ , namely

$$\lim_{r \rightarrow \infty} C_{r,0} \sim \int dq d\Omega q^d e^{i\vec{q} \cdot \vec{r}} \sim \frac{1}{r^{d+1}} \int dq q^{d-1} \sin(q) \sim \frac{1}{r^{d+1}}. \quad (\text{B1})$$

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