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Two-component Bose gas in an optical lattice at single-particle filling

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The Bose-Hubbard model of a twofold degenerate Bose gas is studied in an optical lattice with one particle per site and virtual tunneling to empty and doubly occupied sites. An effective Hamiltonian for this system is derived within a continued-fraction approach. The ground state of the effective model is studied in mean-field approximation for a modulated optical lattice. A dimerized mean-field state gives a Mott insulator whereas the lattice without modulations develops long-range correlated phase fluctuations due to a Goldstone mode. This result is discussed in comparison with the superfluid and the Mott-insulating state of a single-component hard-core Bose gas.

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I. INTRODUCTION

An ultracold Bose gas is brought into an optical lattice, created by a stationary laser field [1]. If the corresponding periodic potential is sufficiently strong, such that tunneling of atoms between the potential wells is strongly suppressed, the phase coherence of the Bose gas is destroyed due to the repulsive interaction between the bosons. In this case the Bose gas becomes a Mott insulator. This ground state is characterized by a fixed number of bosons in each lattice well and strong incoherent phase fluctuations of the quantum state, in contrast to the phase coherence of the Bose-Einstein condensate with a strongly fluctuating local particle number. The Mott insulator and the transition to the superfluid state were discussed theoretically some time ago [2–4] and observed experimentally recently [1].

Besides the phase of the bosons and the local particle number there can be other degrees of freedom in an ultracold gas of bosonic atoms which may also establish some long-range ordering. A possible candidate for such a consideration is a Bose gas in an optical or a magnetic trap [5], where the fluctuations between nearly degenerate hyperfine states represent an additional degree of freedom. This can play a role in establishing different types of ordering, similar to the spin degree of freedom in fermionic systems. Here the case of a strongly interacting Bose gas with one particle per site will be considered. Using a Bose-Hubbard model, the interaction and the chemical potential of a grand-canonical ensemble are adjusted such that there is one particle per optical lattice site. According to the statements given above, the fixed number of particles per site would represent a Mott insulator. On the other hand, the local particle number $n_{\mathbf{r}}$ is a sum of the particle numbers of both components (represented by a "spin" ↑ or ↓)

$$n_{\mathbf{r}}=n_{\mathbf{r},\uparrow}+n_{\mathbf{r},\downarrow}.$$

The individual particle numbers of the two components are fluctuating quantities and can lead to a new state when long-range correlations develop. A similar situation can be found in a single-component hard-core Bose gas in an optical lattice. Then each lattice site is either empty with the quantum state $|0\rangle$ or singly occupied with $|1\rangle$. Formally these two states correspond with the states $|\uparrow\rangle$ and $|\downarrow\rangle$ of the two-component gas. It is known from analytic [2,3] and numerical calculations [6] that the hard-core Bose gas develops a superfluid phase for arbitrarily small tunneling rates if the states $|0\rangle$ and $|1\rangle$ are degenerate, i.e., when $\langle n_{\mathbf{r}}\rangle=1/2$. This behavior will be discussed in Sec. III A. Using the formal correspondence with the two-component Bose gas the development of a long-range correlated state would also take place for any tunneling rate if the states $|\uparrow\rangle$ and $|\downarrow\rangle$ are degenerate. A consequence would be that these two states could easily separate in space, leading to an entangled state in the Bose gas.

Ordering phenomena can be studied perturbatively, starting from isolated potential wells of the optical lattice and systematically turning on the tunneling between these potential wells. Because of the degeneracy with respect to the spin degrees of freedom in the isolated wells this requires a degenerate perturbation theory. Instead of using a perturbation theory for the tunneling Hamiltonian a continued-fraction approach will be applied in the following.

The central aim of this paper is to derive an effective Hamiltonian for the two-component Bose gas with $\langle n_{\mathbf{r}}\rangle=1$ and to discuss the properties of this system. In this case a particle is a superposition of the states $|\uparrow\rangle$ and $|\downarrow\rangle$. Without tunneling between lattice sites it represents a "paramagnetic" state, i.e., a state without ordering. Tunneling, on the other hand, preserves the "spin": starting with a boson of a given spin this boson will spread to neighboring potential wells. This process requires virtual states which are empty or occupied by more than one particle. Here only occupation with two particles will be allowed to keep the calculational effort low. However, the continued-fraction approach proposed in this paper can be extended to higher orders of occupation.

After introducing the two-component Bose-Hubbard model in Sec. II, the single-component hard-core Bose gas is considered for comparison in Sec. III and treated in mean-field approximation in Sec III A. The ground states of a two-component Bose-Hubbard model with $\langle n_{\mathbf{r}}\rangle\leq 1$ and a single-component hard-core Bose gas are evaluated for a two-site system in Sec. III B. Then the effective Hamiltonian for a projected system of interacting particles is derived by a truncated continued fraction in Sec. IV and applied to the two-component Bose gas with $\langle n_{\mathbf{r}}\rangle=1$ in Sec. V. Finally, the two-site system (Sec. V A) and a mean-field approximation (Sec. V B) are discussed for the effective model.

II. THE MODEL: INTERACTING BOSE GAS

In order to describe a multicomponent interacting Bose gas the interaction of bosons can either be included as a hard-core interaction or in terms of the Bose-Hubbard model. Crucial is only that a repulsive interaction stabilizes an incompletely filled lattice with vanishing compressibility. From this point of view the actual form of the local interaction Hamiltonian H_0 is not important except for the fact that it depends only on the local particle number at site $\mathbf{r}$

$$n_{\mathbf{r}}=\sum_{\sigma=\downarrow,\uparrow} a^{\dagger}_{\mathbf{r},\sigma}a_{\mathbf{r},\sigma}$$

with boson creation (annihilation) operator $a^{\dagger}$ (a). For a more specific discussion, a Bose-Hubbard model with

$$H_0=\sum_{\mathbf{r}} [-\mu n_{\mathbf{r}}+Un_{\mathbf{r}}(n_{\mathbf{r}}-1)] \tag{1}$$

shall be considered, where μ is the chemical potential and $U>0$ the interaction constant. Eigenvalues of the local particle number are $n=0,1,\ldots$ with corresponding energies per lattice site

$$E(n)=-\mu n+Un(n-1).$$

For $0<\mu<U$, the case considered throughout this paper, the lowest energy is $E(1)=-\mu$ for $n=1$, and next higher energies are $E(0)=0$ and $E(2)=2(U-\mu)$ and even higher energies for $n>2$.

The dynamics of the bosons is described by the tunneling Hamiltonian

$$H_1=-\sum_{\langle \mathbf{r},\mathbf{r}'\rangle} \tau_{\mathbf{r},\mathbf{r}'}\sum_{\sigma=\downarrow,\uparrow} t_{\sigma}a^{\dagger}_{\mathbf{r},\sigma}a_{\mathbf{r}',\sigma}, \tag{2}$$

where $\langle \mathbf{r},\mathbf{r}'\rangle$ are nearest-neighbor sites on the optical lattice. The parameter $0\leq\tau_{\mathbf{r},\mathbf{r}'}\leq 1$ describes a modulation of the optical lattice. The interaction is crucial for finding new physical states, since the noninteracting Bose gas (i.e., for $U=0$) the Hamiltonian H_1 gives only two independent Bose-Einstein condensates.

A grand-canonical ensemble of bosons at the inverse temperature β, defined by the partition function

$$Z=\mathrm{Tr}\exp(-\beta H), \tag{3}$$

can be used to evaluate the average density of particles as

$$\bar{n}=\frac{1}{\beta N}\frac{\partial ln\, Z}{\partial\mu}$$

with the number of lattice site N. Without tunneling (i.e., for $t_{\sigma}=0$) the average density of particles $\bar{n}$ gives $\partial\bar{n}/\partial\mu=0$ (i.e., incompressible states) for all noninteger values of μ/U.

III. SINGLE-COMPONENT HARD-CORE BOSE GAS: SUPERFLUID AND MOTT-INSULATING STATES

Before discussing the two-component Bose gas the single-component hard-core Bose gas shall be considered because its properties are known from a number of other approaches. The hard-core interaction can be described by a bosonic creation (annihilation) operator $A^{\dagger}$ (A) with the additional condition $A^{\dagger 2}=0$. The Hamiltonian of the hard-core Bose gas then reads

$$H_{\mathrm{HCB}}=-t\sum_{\langle \mathbf{r},\mathbf{r}'\rangle} A^{\dagger}_{\mathbf{r}}A_{\mathbf{r}'}-\mu\sum_{\mathbf{r}} A^{\dagger}_{\mathbf{r}}A_{\mathbf{r}} \tag{4}$$

and acts on the Hilbert space with $|0\rangle$ and $|1\rangle$ as basis states at each lattice site. There is a close formal connection between hard-core Bose and spin-1/2 operators, since one can write

$$S^x=(A+A^{\dagger})/2,\quad S^y=i(A-A^{\dagger})/2,\quad S^z=A^{\dagger}A-1/2. \tag{5}$$

The Hamiltonian can be expressed in terms of these spin operators as an XY model with a magnetic field in z direction:

$$H_{\mathrm{HCB}}=-t\sum_{\langle \mathbf{r},\mathbf{r}'\rangle} (S^x_{\mathbf{r}}S^x_{\mathbf{r}'}+S^y_{\mathbf{r}}S^y_{\mathbf{r}'})-\mu\sum_{\mathbf{r}} S^z_{\mathbf{r}}.$$

For sufficiently large values of $|\mu|$ the ground state is ferromagnetic: if $\mu>0$ the magnetization is $\langle S^z\rangle>0$ and vice versa. Therefore, for $\mu>0$ $(\mu<0)$ these ground states correspond in terms of the hard-core bosons with a completely filled (empty) lattice, where the filled lattice represents a Mott-insulating state [2–4]. $\mu=0$ is a marginal situation, where the bosons develop a superfluid state for any positive value of the tunneling rate t. More general, the superfluid state persists if the tunneling dominates.

The advantage of the spin representation is that it provides a simple qualitative picture for the existence of a Mott-insulating state and a transition to a superfluid state. A more quantitative description is obtain from a mean-field approximation which is discussed in the following section.

A. Mean-field approximation of the hard-core Bose gas

A possible complex mean-field state for the hard-core Bose gas is

$$|\Psi_{MF}\rangle=\prod_{\mathbf{r}} [e^{i\varphi_{\mathbf{r}}}\cos(\eta_{\mathbf{r}})+e^{i\psi_{\mathbf{r}}}\sin(\eta_{\mathbf{r}})A^{\dagger}_{\mathbf{r}}]|0\rangle \tag{6}$$

from which matrix elements can be calculated. For instance, the tunneling term in the Hamiltonian H_{HCB} gives

$$\langle\Psi_{MF}|A^{\dagger}_{\mathbf{r}}A_{\mathbf{r}'}+A^{\dagger}_{\mathbf{r}'}A_{\mathbf{r}}|\Psi_{MF}\rangle$$
$$=2\cos(\alpha_{\mathbf{r}}-\alpha_{\mathbf{r}'})\cos(\eta_{\mathbf{r}})\sin(\eta_{\mathbf{r}})\cos(\eta_{\mathbf{r}'})\sin(\eta_{\mathbf{r}'}),$$

where the phases appear only in the phase difference $\alpha_{\mathbf{r}}=\varphi_{\mathbf{r}}-\psi_{\mathbf{r}}$. Thus this term of the Hamiltonian has a global

U(1) symmetry because it is invariant under a shift $\varphi_{\mathbf{r}}\to\varphi_{\mathbf{r}}+\Delta$ and $\psi_{\mathbf{r}}\to\psi_{\mathbf{r}}+\Delta'$. The other matrix element of the Hamiltonian $H_{\rm HCB}$ is independent of the phases:

$$\langle\Psi_{MF}|A_{\mathbf{r}}^\dagger A_{\mathbf{r}}|\Psi_{MF}\rangle=\sin^2\eta_{\mathbf{r}}.$$

The mean-field expectation of Hamiltonian (4) with the homogeneous mean field η reads

$$\langle\Psi_{MF}|H_{\rm HCB}|\Psi_{MF}\rangle=-\sin^2\eta\left[t(1-\sin^2\eta)\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}\cos(\alpha_{\mathbf{r}}-\alpha_{\mathbf{r}'})+\sum_{\mathbf{r}}\mu\right].$$

The ground state is $\cos(\alpha_{\mathbf{r}}-\alpha_{\mathbf{r}'})=1$ and

$$\sin^2\eta=\begin{cases}0 & \text{for}\quad \mu\leqslant-2dt\\ 1/2+\mu/4dt & \text{for}\quad -2dt<\mu<2dt\\ 1 & \text{for}\quad 2dt\leqslant\mu.\end{cases}\qquad(7)$$

The expression

$$\langle\Psi_{MF}|A_{\mathbf{r}}|\Psi_{MF}\rangle=e^{i(\psi_{\mathbf{r}}-\varphi_{\mathbf{r}})}\cos\eta\sin\eta\qquad(8)$$

is an order parameter for a superfluid state which vanishes in the cases $\sin^2\eta=0,1$. It should be noticed that in this regime $\langle\Psi_{MF}|H_{\rm HCB}|\Psi_{MF}\rangle$ is independent of $\alpha_{\mathbf{r}}$. This reflects the absence of a superfluid. In the case $\sin^2\eta=0$ it is an empty state and for $\sin^2\eta=1$ a Mott insulator with one particle per site. This result is in agreement with Monte Carlo simulations [6].

B. Hard-core vs Bose-Hubbard model: A two-site system

To study the tunneling between neighboring potential wells of the optical lattice a two-site model with $t_\uparrow=t_\downarrow\equiv t$ is considered. This was already discussed in great detail for the model under consideration, using the leading order of an expansion in t^2/U [7–9]. Here the study shall be performed without assuming $t^2/U\ll1$. As a first example the single-component hard-core Bose gas is considered in terms of the Hamiltonian in Eq. (4). The ground states are

$$|\Psi_0\rangle=\begin{cases}|0,0\rangle & \text{for } \mu<-t\\ (|0,1\rangle+|1,0\rangle)/\sqrt{2} & \text{for } -t<\mu<t\\ |1,1\rangle & \text{for } \mu>t.\end{cases}$$

This result corresponds with the three different mean-field ground states in Eq. (7). Thus already the two-site system indicates the three phases of the full d-dimensional lattice: the empty lattice, the condensate, and the $n=1$ Mott insulator. An analogous calculation for the two-component Bose-Hubbard model with empty and singly occupied sites gives the ground states

$$|\Psi_0\rangle=\begin{cases}|0,0\rangle & \text{for } \mu<-t\\ (|0,\uparrow\rangle+|\uparrow,0\rangle)/\sqrt{2},\quad(|0,\downarrow\rangle+|\downarrow,0\rangle)/\sqrt{2} & \text{for } -t<\mu<t\\ |\downarrow,\downarrow\rangle,|\downarrow,\uparrow\rangle,|\uparrow,\downarrow\rangle,|\uparrow,\uparrow\rangle & \text{for } \mu>t.\end{cases}\qquad(9)$$

For $-t<\mu<t$ there are two (degenerate) ferromagnetic states, where the degeneracy can be lifted by an infinitesimal magnetic field. It is expected that these are the states which form a condensate. The fourfold degeneracy for $\mu>t$ may be lifted when a virtual tunneling through empty and doubly occupied sites is included. This degeneracy also raises the question whether or not an analog of the superfluid ground state is allowed due to virtual tunneling in this regime. A reason for having long-range correlations is that one of the two components, e.g., $|\downarrow\rangle$, can be formally considered as an empty site, the other component as a hard-core boson and since the hard-core Bose gas has a superfluid state for sufficiently large tunneling rate. To study this regime, a projection of the trace in the partition function to singly occupied states is considered subsequently. This projection allows virtual tunneling through empty and doubly occupied sites.

IV. A CONTINUED-FRACTION APPROACH TO THE PROJECTED PARTITION FUNCTION

The many-body system is defined by the Hamiltonian H and the transfer matrix e^{-H}. Physical quantities at inverse temperature β are derived from the partition function Z defined in Eq. (3). A continued-fraction approach shall be developed in this section to derive an effective Hamiltonian from H that describes the physics of a projected transfer matrix $P_0e^{-\beta H}P_0$. Although H is bounded from below it may have negative eigenvalues. A positive operator can be obtained by adding a constant diagonal term E to shift the ground-state energy E_0 to positive values $E(1)=E_0+E$. Then the transfer matrix can be represented by the integral

$$e^{-\beta H}=\frac{e^{\beta E}}{2\pi i}\int_{-\infty}^{\infty}e^{i\beta z}[z-i(H+E)]^{-1}dz.$$

Thermodynamic properties at low temperatures are dominated by the ground states and low-energy excitations. The trace of the grand-canonical partition function Z includes states with all possible number of bosons. For the Hamiltonian H the highest statistical weight comes from the ground state. If $H=H_0+H_1$ with a perturbation H_1, the Hilbert space is projected on the degenerate ground states of the Hamiltonian H_0 by P_0. In the example of Sec. II the Hamiltonian preserves the number of particles. Therefore, in this case it is expected that the system with fixed particle filling gives the dominant contribution to the trace, especially at low temperatures. This situation can be described by the P_0-projected partition function with the corresponding trace Tr_0

$$Z=\mathrm{Tr}_0(P_0e^{-\beta H}P_0)$$
$$=\frac{e^{\beta E}}{2\pi i}\int_{-\infty}^{\infty}e^{i\beta z}\mathrm{Tr}_0[P_0\{z-i(H+E)\}^{-1}P_0]dz. \quad (10)$$

Assuming that H is implicitly shifted by E, the P_0 projection of the resolvent $(z-iH)^{-1}$ reads

$$P_0(z-iH)^{-1}P_0$$
$$=[P_0(z-iH)P_0+P_0HP_1(z-iH)_1^{-1}P_1HP_0]_0^{-1}, \quad (11)$$

with $P_1=\mathbf{1}-P_0$. $(\cdots)_{0,1}^{-1}$ is the inverse with respect to the $P_{0,1}$-projected space. This identity can be directly shown by a multiplication of the matrix and its inverse. It can be generalized to a recurrence relation [see Eq. (A2) of Appendix A] if the Hamiltonian H satisfies the special conditions (A1). For the two-component Bose gas this is indeed the case, since the Hamiltonian $H=H_0+H_1$ of Sec. II is of the special form

$$H=\begin{pmatrix} P_0H_0P_0 & P_0H_1P_1 \\ P_1H_1P_0 & P_1HP_1 \end{pmatrix}, \quad (12)$$

where P_0 is the projection to the degenerate ground state of H_0 with $0<\mu<U$, i.e., one particle per site. Thus the Hamiltonian H_1 is responsible for an interaction between the P_0- and the P_1-projected Hilbert spaces. H_0, on the other hand, acts only inside the P_0-projected space. Starting from singly occupied states, the tunneling Hamiltonian H_1 can only create a pair of an empty and a doubly occupied site (PEDS). If P_2 is the projection from P_1 to one with only a single PEDS, the second term in the inverse matrix of Eq. (11) reads

$$P_0H_1P_1(z-iH)_1^{-1}P_1H_1P_0=P_0H_1P_2(z-iH)_1^{-1}P_2H_1P_0. \quad (13)$$

In general, the operator $P_{2k+1}H_1P_{2k}$ creates a new PEDS in the Hilbert space with k PEDSs. Thus the continued-fraction representation of Appendix A, applied to the two-component Bose gas at single-particle filling, is based on the creation of PEDSs.

In order to truncate the continued fraction the creation of new PEDS and multiply occupied sites is excluded. This is related to the approximation

$$P_2(z-iH)_1^{-1}P_2\approx P_2(z-iH_0)_1^{-1}P_2$$
$$=\frac{1}{z-i[(N-2)E(1)+E(0)+E(2)]}P_2,$$

where $E(0)$ and $E(2)$ are the energies of H_0+E for the empty and doubly occupied sites of Sec. II. With Eqs. (11) and (13) this gives for the P_0-projected resolvent of the partition function

$$P_0(z-iH)^{-1}P_0\approx\{P_0(z-iH_0)P_0+P_0H_1P_2$$
$$\times[z-iH_0]^{-1}P_2H_1P_0\}_0^{-1}$$
$$=(z-iE_0+P_0H_1^2P_0/\{z-i[(N-2)E(1)$$
$$+E(0)+E(2)]\})_0^{-1}.$$

Here it has been used that

$$P_0H_1P_2H_1P_0=P_0H_1^2P_0,$$

which follows from the fact that H_1 is off-diagonal with respect to the P_0- and P_2-projected Hilbert spaces. Then the P_0-projected partition function reads for low temperatures (i.e., $\beta\sim\infty$) (see Appendix B)

$$Z\sim\tfrac{1}{2}e^{-\beta(NE_0+\Delta E)}\mathrm{Tr}_0[e^{-\beta H_{eff}}(1-\Delta EH_{eff}^{-1})], \quad (14)$$

with the effective Hamiltonian

$$H_{eff}=-[(\Delta E)^2+P_0H_1^2P_0]^{1/2}=-\Delta E[1$$
$$+P_0H_1^2P_0/(\Delta E)^2]^{1/2}$$

and

$$\Delta E=[E(0)+E(2)]/2-E(1).$$

Since $P_0H_1^2P_0$ is a non-negative operator, this result implies that the ground state of $-P_0H_1^2P_0$ is the ground state of H_{eff}.

If $P_0H_1^2P_0$ is small in comparison with $(\Delta E)^2$, a perturbation theory with respect to the $P_0H_1^2P_0$ can be applied to H_{eff}. This leads to an expansion with respect to t^2/U. In leading order the approximation is

$$H_{eff}\approx-\Delta E-P_0H_1^2P_0/(2\Delta E),$$

in agreement with the results of Refs. [7–9].

This method of deriving an effective Hamiltonian by projecting the partition function is quite general as long as the Hamiltonian H has the structure shown in Eq. (12). The specific case of a two-component Bose gas will be discussed subsequently.

V. THE EFFECTIVE HAMILTONIAN OF THE PROJECTED TWO-COMPONENT BOSE GAS

Numerous possibilities were discussed in the literature for the creation of a two-component system in atomic gases [10–13]. For instance, if ^{87}Rb is coupled to a radiation field there are pairs of nearly degenerate hyperfine $|F,m_F\rangle$ states, namely, $|\uparrow\rangle=|1,-1\rangle$ and $|\downarrow\rangle=|2,1\rangle$ [10,14] or $|\uparrow\rangle=|1,-1\rangle$ and $|\downarrow\rangle=|2,-2\rangle$ [12]. $|\downarrow\rangle$ and $|\uparrow\rangle$ are formal notations to specify the two (almost) degenerate states. The interaction of the atoms does not depend on the states but only on the local density of the bosons. Therefore, the interaction in H_0 of Eq. (1) is a good description.

In a dilute regime (i.e., for a filling less than one particle per site) the interaction is weak. This opens the opportunity to apply a classical approach for the two-component condensate order parameter, leading to a lattice version of the Gross-Pitaevskii equation. The optical lattice means that the kinetic term has a special band dispersion $\epsilon(\mathbf{k})$ in Fourier space, depending on the lattice, instead of the k^2 dispersion in the case without an optical lattice. It is believed that this model has a ferromagnetic ground state with respect to the two-component bosons [15], a result that is also supported by the result of the two-site system in Eq. (9). On the other hand, it is well known from the theory of the fermionic Hubbard model that the type of spin order depends crucially on the filling of the lattice [16,17], and can change, for instance, from ferromagnetic to antiferromagnetic order by changing the filling. In particular, the fermionic Hubbard model has an antiferromagnetic ground state at half filling. To study this effect in the two-component Bose gas in an optical lattice, the strongly interacting case with single-particle filling of the lattice shall be considered here. Then the two-component degeneracy has to be taken fully into account and the projection approach of the preceding secion for the tunneling term H_1 should be applied. In this case the Hamiltonian $-P_0H_1^2P_0$ reads

$$-\frac{1}{4}\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}\tau^2_{\mathbf{r},\mathbf{r}'}\sum_{\sigma,\sigma'=\downarrow,\uparrow}t_\sigma t_{\sigma'}P_0(a^\dagger_{\mathbf{r},\sigma}a_{\mathbf{r}',\sigma}+a^\dagger_{\mathbf{r}',\sigma}a_{\mathbf{r},\sigma})\times(a^\dagger_{\mathbf{r},\sigma'}a_{\mathbf{r}',\sigma'}+a^\dagger_{\mathbf{r}',\sigma'}a_{\mathbf{r},\sigma'})P_0 \tag{15}$$

and $\Delta E=U$. On the P_0-projected Hilbert space (i.e., the space with exactly one particle per site) the operators

$$A^\dagger_{\mathbf{r}}=P_0a^\dagger_{\mathbf{r},\uparrow}a_{\mathbf{r},\downarrow}P_0,\quad A_{\mathbf{r}}=P_0a^\dagger_{\mathbf{r},\downarrow}a_{\mathbf{r},\uparrow}P_0$$

are creation and annihilation operators of hard-core bosons, when $|\downarrow\rangle$ is formally identified with a vacuum state $|0\rangle$ and $|\uparrow\rangle$ with a one-particle state $|1\rangle$. As shown in Appendix C, the operator $-P_0H_1^2P_0$ reads in terms of the hard-core Bose operators as

$$-P_0H_1^2P_0=-\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}\tau^2_{\mathbf{r},\mathbf{r}'}\left[t_\uparrow t_\downarrow A^\dagger_{\mathbf{r}}A_{\mathbf{r}'}+\frac{t_\uparrow^2+t_\downarrow^2}{2}\times(\mathbf{1}-A^\dagger_{\mathbf{r}}A_{\mathbf{r}})A^\dagger_{\mathbf{r}'}A_{\mathbf{r}'}\right]. \tag{16}$$

This Hamiltonian describes a hard-core Bose gas with a repulsive nearest-neighbor interaction. The competition between tunneling (favors particles) and nearest-neighbor repulsion (favors a ground state with checkerboard order) leads to a complex situation. Similar to the single-component hard-core Bose gas, this can also be discussed in terms of spin-1/2 states. The representation of Hamiltonian (16) as a spin Hamiltonian via Eq. (5) gives an anisotropic Heisenberg Hamiltonian.

A. Projected two-site model

The situation of the projected partition function of the two-site model can be discussed and compared with the previous results for the hard-core Bose gas and the two-component Bose-Hubbard gas. Using the hard-core Bose Hamiltonian of the projected model in Eq. (16) with $t_\uparrow=t_\downarrow\equiv t$ and $\tau_{\mathbf{r},\mathbf{r}'}=1$, the corresponding 4×4 matrix for the four different states with $\downarrow$ and $\uparrow$ at the two sites has the eigenvalues $\{-2t^2,0,0,0\}$. The unique ground state of $-P_0H_1^2P_0$ with energy $-2t^2$ is

$$|\Psi_0\rangle=\frac{1}{\sqrt{2}}(|\downarrow,\uparrow\rangle+|\uparrow,\downarrow\rangle). \tag{17}$$

The P_0 projection has apparently selected a nondegenerate ground state from the four degenerate ground states of the Bose-Hubbard model with one particle per site in Eq. (9). This is a consequence of the virtual tunneling to empty and doubly occupied states in the model with the projected partition function, which was not included in the derivation of the state $|\Psi_0\rangle$ of Eq. (9). This state is not an eigenstate to $S^z_{\mathbf{r}}$ but has a vanishing expectation for $S^z_{\mathbf{r}}$. This reflects the fact that the ground state has no tendency to develop a ferromagnetic order.

The projected partition function (14) reads for this two-site model

$$Z\sim e^{-\beta(2E_0+U)}\sum_{j=1}^{4}e^{\beta(U^2-E_j)^{1/2}}\sim e^{-\beta(2E_0+U)}e^{\beta(U^2+2t^2)^{1/2}}.$$

Z can be used to evaluate the average tunneling energy from

$$\frac{t}{\beta}\frac{\partial}{\partial t}\ln Z\sim\frac{2t^2}{\sqrt{U^2+2t^2}}.$$

Thus the interaction reduces the tunneling rate of the two-site model by a factor $(1+U^2/2t^2)^{-1/2}$.

B. Mean-field approximation of the two-component Bose gas

Using the hard-core Bose representation of the Hamiltonian in Eq. (16) its mean-field approximation is studied with the complex mean-field state (6). The repulsive nearest-neighbor interaction is

$$\langle\Psi_{MF}|(\mathbf{1}-A^\dagger_{\mathbf{r}}A_{\mathbf{r}})A^\dagger_{\mathbf{r}'}A_{\mathbf{r}'}|\Psi_{MF}\rangle=\cos^2\eta_{\mathbf{r}}\sin^2\eta_{\mathbf{r}'}.$$

Together with the hard-core Bose Hamiltonian of Sec. III A the expression in the Hamiltonian of the two-component Bose gas at single filling reads in mean-field approximation

$$-\langle\Psi_{MF}|P_0H_1^2P_0|\Psi_{MF}\rangle=-\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}\tau^2_{\mathbf{r},\mathbf{r}'}\left[t_\uparrow t_\downarrow\cos(\alpha_{\mathbf{r}}-\alpha_{\mathbf{r}'})\cos\eta_{\mathbf{r}}\sin\eta_{\mathbf{r}}\cos\eta_{\mathbf{r}'}\times\sin\eta_{\mathbf{r}'}+\frac{t_\uparrow^2+t_\downarrow^2}{2}\cos^2\eta_{\mathbf{r}}\sin^2\eta_{\mathbf{r}'}\right].$$

The first term favors a homogeneous solution for $\eta_{\mathbf{r}}$, the second term an inhomogeneous solution, e.g., for neighboring sites $\mathbf{r},\mathbf{r}'$ with

$$\sin^2\eta_{\mathbf{r}}=1, \quad \cos^2\eta_{\mathbf{r}'}=1. \tag{18}$$

In this case the first term vanishes and the remaining Hamiltonian is

$$-\langle\Psi_{MF}|P_0H_1^2P_0|\Psi_{MF}\rangle_i=-\frac{t_\uparrow^2+t_\downarrow^2}{4}\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}\tau_{\mathbf{r},\mathbf{r}'}^2 .$$

On the other hand, a homogeneous mean-field solution for the ground state is $\sin^2\eta=1/2$ such that

$$-\langle\Psi_{MF}|P_0H_1^2P_0|\Psi_{MF}\rangle_h$$
$$=-\frac{1}{4}\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}\tau_{\mathbf{r},\mathbf{r}'}^2\left[t_\uparrow t_\downarrow\cos(\alpha_{\mathbf{r}}-\alpha_{\mathbf{r}'})+\frac{t_\uparrow^2+t_\downarrow^2}{2}\right]. \tag{19}$$

This Hamiltonian agrees formally with the mean-field Hamiltonian of hard-core bosons in Sec. III A at the point of degeneracy $\mu=0$. However, its interpretation in terms of the physical bosons, given by the Bose operators $a^\dagger$ and a, is different. This is clearly indicated by the fact that the order parameter of a superfluid state vanishes:

$$\langle\Psi_{MF}|a_{\mathbf{r}}|\Psi_{MF}\rangle_h=0.$$

Thus the long-range correlated phase fluctuations are not related to a superfluid state but to a spontaneously broken symmetry, associated with the order parameter

$$\langle\Psi_{MF}|A_{\mathbf{r}}|\Psi_{MF}\rangle_h=\langle\Psi_{MF}|a_{\mathbf{r},\downarrow}^\dagger a_{\mathbf{r},\uparrow}|\Psi_{MF}\rangle_h .$$

These phase fluctuations prevent the system to become a genuine Mott insulator, since the latter is characterized by a gap and short-range correlated fluctuations (cf. with the Mott-insulating state of the single-component hard-core gas in Sec. III A). However, a Mott insulator can be obtained in the limit $t_\uparrow t_\downarrow=0$. This is a limit similar to the Falicov-Kimball limit of the fermionic Hubbard model [17].

Another mean-field approximation can be constructed for a generalization of the two-site model to a modulated lattice model, using dimers with tunneling rates $\tau_{\mathbf{r},\mathbf{r}'}=\tau_0$ as building blocks of the lattice. These dimers are weakly coupled with tunneling rate $\tau_{\mathbf{r},\mathbf{r}'}=\tau_1\ll\tau_0$. A corresponding complex mean-field state is

$$|\Psi_D\rangle=\prod_{\langle\mathbf{r},\mathbf{r}'\rangle\in D}\frac{1}{\sqrt{2}}(e^{i\varphi_{\mathbf{r}}}A_{\mathbf{r}}^\dagger+e^{i\varphi_{\mathbf{r}'}}A_{\mathbf{r}'}^\dagger)|0\rangle, \tag{20}$$

where D is a set of dimers $\{\langle\mathbf{r},\mathbf{r}'\rangle\}$ with $\tau_{\mathbf{r},\mathbf{r}'}=\tau_0$. This state is a lattice generalization of the two-site state of Eq. (17). The Hamiltonian of the two-component Bose gas at single filling (16) reads in this mean-field approximation

$$-\langle\Psi_D|P_0H_1^2P_0|\Psi_D\rangle$$
$$=-\frac{\tau_0^2}{2}t_\uparrow t_\downarrow\sum_{\langle\mathbf{r},\mathbf{r}'\rangle\in D}\cos(\varphi_{\mathbf{r}}-\varphi_{\mathbf{r}'})-\frac{t_\uparrow^2+t_\downarrow^2}{4}\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}\tau_{\mathbf{r},\mathbf{r}'}^2 . \tag{21}$$

For $t_\uparrow t_\downarrow=0$ this result agrees with the Hamiltonian of solution (18) but has a lower energy for any $t_\uparrow t_\downarrow>0$. Moreover, the state $|\Psi_D\rangle$ has always a lower energy than the homogeneous mean-field state $|\Psi_{MF}\rangle_h$. This can be summarized by comparing the ground-state energies: The difference between the ground-state energy of the homogeneous (E_h) state $|\Psi_{MF}\rangle_h$ and the inhomogeneous (E_i) state $|\Psi_{MF}\rangle_i$ is

$$E_h-E_i=\frac{(t_\uparrow-t_\downarrow)^2}{8}\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}\tau_{\mathbf{r},\mathbf{r}'}^2$$

and between the inhomogeneous state $|\Psi_{MF}\rangle_i$ and the dimerized state $|\Psi_D\rangle$ is

$$E_i-E_D=\frac{t_\uparrow t_\downarrow}{2}\sum_{\langle\mathbf{r},\mathbf{r}'\rangle\in D}\tau_{\mathbf{r},\mathbf{r}'}^2 .$$

It should be noticed that the homogeneous state $|\Psi_{MF}\rangle_h$ and the dimerized state $|\Psi_D\rangle$ have the same ground-state energy in the case of a single-component hard-core Bose gas, provided that the dimers fill half of the lattice. This means that the difference of the ground-state energies in the Hamiltonian of Eq. (16) is due to the repulsive interaction.

The Hamiltonian of Eq. (21) creates short-range correlated fluctuations, since the set D contains only isolated dimers. Therefore, it represents a Mott insulator. If the modulation of the lattice is weak (i.e., $\tau_0\approx\tau_1$), a summation of the state in Eq. (20) over different dimer configurations is required. This may lead again to long-range correlated phase fluctuations, since the global U(1) symmetry of the phase fluctuations can be spontaneously broken. Thus a phase transition from a Mott insulator at strong modulation to a state with long-range correlated phase fluctuations at weak modulation is expected.

VI. SUMMARY

A two-component Bose gas with creation operators $a_\uparrow^\dagger$, $a_\downarrow^\dagger$ in an optical lattice with lattice modulations and one particle per site is studied. By allowing only virtual tunneling to empty and doubly occupied sites, an effective Hamiltonian is derived for hard-core bosons, defined by the creation operator

$$A^\dagger=P_0a_{\mathbf{r},\uparrow}^\dagger a_{\mathbf{r},\downarrow}P_0 ,$$

where P_0 is the projector on one-particle states. The effective Hamiltonian describes tunneling and a repulsive nearest-neighbor interaction between hard-core bosons. It is studied in terms of two types of mean-field states: a product of single-particle states and a dimerized state. The ground-state energies of a homogeneous single-particle product state

(E_h), of a inhomogeneous single-particle product state (E_i), and of a dimerized state (E_D) are related as

$$E_D \leqslant E_i \leqslant E_h,$$

where the first equality sign holds for $t_\uparrow t_\downarrow = 0$ and the second for $t_\uparrow = t_\downarrow$.

The repulsive nearest-neighbor interaction prefers the dimerized state, indicating a Mott insulator at least in the presence of a lattice modulation. This state is characterized by short-range correlated phase fluctuations. For small or even vanishing modulation, however, a superposition of different dimerized states may lead to a spontaneously broken U(1) symmetry of the phase fluctuations. This would be accompanied by a Goldstone mode with long-range correlated phase fluctuations, indicating the destruction of the Mott insulator and the creation of an ordered state in terms of the two components of the Bose gas.

A similar model with N components and hard-core interaction was studied in the $N \to \infty$ limit [18]. It has a Mott-insulating phase with $\bar{n} = 1$ and indicates a symmetry-breaking phase for $0 < \bar{n} < 1$.

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APPENDIX A

Given is a sequence of projectors $P_j (j \geqslant 0)$, defined by

$$P_{2k+1} = P_{2k-1} - P_{2k} \quad (k \geqslant 0)$$

with initial condition $P_{-1} = \mathbf{1}$ and with the Hamiltonian H through the properties

$$P_{2k} H P_{2k+1} = P_{2k} H P_{2k+2}, \quad P_{2k+1} H P_{2k} = P_{2k+2} H P_{2k}. \tag{A1}$$

With these projectors the identity, Eq. (11), can be iterated. The first step is to replace $P_0 H P_1 (z - iH)_1^{-1} P_1 H P_0$ by the right-hand side of the identity

$$P_0 H P_1 (z - iH)_1^{-1} P_1 H P_0 = P_0 H P_2 (z - iH)_1^{-1} P_2 H P_0,$$

such that Eq. (11) reads

$$P_0 (z - iH)^{-1} P_0 = [P_0 (z - iH) P_0 + P_0 H P_2 (z - iH)_1^{-1} P_2 H P_0]_0^{-1}.$$

Now the expression $P_2 (z - iH)_1^{-1} P_2$ on the right-hand side can be rewritten by applying again Eq. (11) as

$$P_2 (z - iH)_1^{-1} P_2 = [P_2 (z - iH) P_2 + P_2 H P_3 (z - iH)_3^{-1} P_3 H P_2]_2^{-1},$$

with $P_3 = P_1 - P_2$. Moreover, application of Eq. (A1) to the right-hand side yields

$$P_2 (z - iH)_1^{-1} P_2 = [P_2 (z - iH) P_2 + P_2 H P_4 (z - iH)_3^{-1} P_4 H P_2]_2^{-1}.$$

Iteration of this procedure leads to the recurrence relation

$$P_{2k} (z - iH)_{2k-1}^{-1} P_{2k} = [P_{2k} (z - iH) P_{2k} + P_{2k} H P_{2k+2} \times (z - iH)_{2k+1}^{-1} P_{2k+2} H P_{2k}]_{2k}^{-1}. \tag{A2}$$

Together with Eq. (11) this gives a continued-fraction representation of $P_0 (z - iH)^{-1} P_0$.

APPENDIX B

To evaluate integral (10) it is convenient to define

$$E_1 = \frac{2}{N} \Delta E + E(1), \quad \Delta E = [E(0) + E(2)]/2 - E(1).$$

Moreover, the spectral representation of $P_0 H_1^2 P_0$ is used with the eigenvalues λ_j. This leads to

$$Z = \sum_j I(\lambda_j),$$

with the integral

$$I(\lambda) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{e^{i\beta z}(z - iNE_1)}{[z - iNE(1)](z - iNE_1) + \lambda} dz.$$

The poles of the integrand are

$$z_\pm = \frac{i}{2} \{ N[E(1) + E_1] \pm \sqrt{N^2 [E_1 - E(1)]^2 + 4\lambda} \},$$

such that the integral itself is

$$I(\lambda) = \frac{e^{i\beta z_+}(z_+ - iNE_1) - e^{i\beta z_-}(z_- - iNE_1)}{z_+ - z_-}.$$

The second term of the numerator dominates at large values β:

$$I(\lambda) \sim - \frac{e^{i\beta z_-}(z_- - iNE_1)}{z_+ - z_-}. \tag{B1}$$

Since

$$z_+ - z_- = i \sqrt{N^2 [E_1 - E(1)]^2 + 4\lambda},$$

$$z_- - iNE_1 = \frac{i}{2} \{ N[E(1) - E_1] - \sqrt{N^2 (E_1 - E_0)^2 + 4\lambda} \}$$

and

$$E_1 - E(1) = \frac{2}{N} \Delta E,$$

the expression in Eq. (B1) reads

$$I(\lambda)\sim\frac{1}{2}e^{-\beta(NE(1)+\Delta E)}e^{\beta\sqrt{(\Delta E)^2+\lambda}}\left[1+\frac{\Delta E}{\sqrt{(\Delta E)^2+\lambda}}\right].$$

APPENDIX C

It is convenient to split the summation $\Sigma_{\sigma,\sigma'}$ in Eq. (15) into a diagonal part and an off-diagonal part:

$$-P_0H_1^2P_0=-\frac{1}{2}\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}\tau_{\mathbf{r},\mathbf{r}'}^2\Bigg[\sum_{\sigma=\downarrow,\uparrow}t_\sigma^2P_0a_{\mathbf{r},\sigma}^\dagger a_{\mathbf{r},\sigma}a_{\mathbf{r}',\sigma}a_{\mathbf{r}',\sigma}^\dagger P_0 +2t_\uparrow t_\downarrow P_0a_{\mathbf{r},\downarrow}^\dagger a_{\mathbf{r},\uparrow}a_{\mathbf{r}',\uparrow}^\dagger a_{\mathbf{r}',\downarrow}P_0\Bigg].$$

The projection P_0 acts individually at each lattice site $\mathbf{r}$, i.e., for $\mathbf{r}'\neq\mathbf{r}$ one can write

$$P_0a_{\mathbf{r},\sigma}^\dagger a_{\mathbf{r},\sigma}a_{\mathbf{r}',\sigma}a_{\mathbf{r}',\sigma}^\dagger P_0=P_0a_{\mathbf{r},\sigma}^\dagger a_{\mathbf{r},\sigma}P_0P_0a_{\mathbf{r}',\sigma}a_{\mathbf{r}',\sigma}^\dagger P_0$$

and

$$P_0a_{\mathbf{r},\sigma}^\dagger a_{\mathbf{r},\sigma'}a_{\mathbf{r}',\sigma'}^\dagger a_{\mathbf{r}',\sigma}P_0=P_0a_{\mathbf{r},\sigma}^\dagger a_{\mathbf{r},\sigma'}P_0P_0a_{\mathbf{r}',\sigma'}^\dagger a_{\mathbf{r}',\sigma}P_0.$$

With this it is possible to define operators on the P_0-projected Hilbert space (i.e., the space with one particle per site) as

$$A_{\mathbf{r}}^\dagger=P_0a_{\mathbf{r},\uparrow}^\dagger a_{\mathbf{r},\downarrow}P_0,\quad A_{\mathbf{r}}=P_0a_{\mathbf{r},\downarrow}^\dagger a_{\mathbf{r},\uparrow}P_0.$$

When $|\downarrow\rangle$ is formally identified with a vacuum state and $|\uparrow\rangle$ with a particle, $A^\dagger$ (A) is a creation (annihilation) operator for a hard-core boson on the P_0-projected Hilbert space. Moreover, it is

$$P_0a_{\mathbf{r},\sigma}a_{\mathbf{r},\sigma}^\dagger P_0=P_0-P_0a_{\mathbf{r},\sigma}^\dagger a_{\mathbf{r},\sigma}P_0, \tag{C1}$$

and the operators satisfy the identities

$$A_{\mathbf{r}}^\dagger A_{\mathbf{r}}=P_0a_{\mathbf{r},\uparrow}^\dagger a_{\mathbf{r},\downarrow}P_0a_{\mathbf{r},\downarrow}^\dagger a_{\mathbf{r},\uparrow}P_0 =P_0a_{\mathbf{r},\uparrow}^\dagger a_{\mathbf{r},\uparrow}P_0=P_0a_{\mathbf{r},\downarrow}a_{\mathbf{r},\downarrow}^\dagger P_0, \tag{C2}$$

$$A_{\mathbf{r}}A_{\mathbf{r}}^\dagger=P_0a_{\mathbf{r},\downarrow}^\dagger a_{\mathbf{r},\uparrow}P_0a_{\mathbf{r},\uparrow}^\dagger a_{\mathbf{r},\downarrow}P_0 =P_0a_{\mathbf{r},\downarrow}^\dagger a_{\mathbf{r},\downarrow}P_0=P_0a_{\mathbf{r},\uparrow}a_{\mathbf{r},\uparrow}^\dagger P_0. \tag{C3}$$

Thus $A_{\mathbf{r}}^\dagger A_{\mathbf{r}}$ is the particle number operator for the hard-core bosons. With (C1) and (C2) the Hamiltonian $-P_0H_1^2P_0$ can be written in terms of the hard-core Bose operators as

$$-P_0H_1^2P_0=-\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}\tau_{\mathbf{r},\mathbf{r}'}^2\left[t_\uparrow t_\downarrow A_{\mathbf{r}}^\dagger A_{\mathbf{r}'} +\frac{t_\uparrow^2+t_\downarrow^2}{2}(\mathbf{1}-A_{\mathbf{r}}^\dagger A_{\mathbf{r}})A_{\mathbf{r}'}^\dagger A_{\mathbf{r}'}\right].$$

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