Commensurate Two-Component Bosons in an Optical Lattice: Ground State Phase Diagram

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(Received 25 June 2003; published 3 February 2004)

Two sorts of bosons in an optical lattice at commensurate filling factors can form five stable superfluid and insulating ground states with rich and nontrivial phase diagram. The structure of the ground state diagram is established by mapping a d-dimensional quantum system onto a $(d+1)$-dimensional classical loop-current model and Monte Carlo (MC) simulations of the latter. Surprisingly, the quantum phase diagram features, besides second-order lines, first-order transitions and two multicritical points. We explain why first-order transitions are generic for models with pairing interactions using microscopic and mean-field (MF) arguments. In some cases, the MC results strongly deviate from the MF predictions.

DOI: 10.1103/PhysRevLett.92.050402 PACS numbers: 03.75.Kk, 05.30.Jp

Ultracold atoms trapped in an optical lattice (OL) [1,2] form an intriguing strongly correlated quantum system. The unprecedented control over parameters of the effective Hubbard-type Hamiltonian renders this system an important object for the study of quantum phase transitions [3]. Single-component bosons without internal degrees of freedom have only two phases in a regular lattice: superfluid (SF) and Mott insulator (MI) (at commensurate filling factor [4]). When several bosonic species are combined in the OL, the naive expectation that their ground states are straightforward mixtures of MI and SF with respect to participating components is wrong — the phases of spinor and multicomponent systems are far more subtle [5–10].

In this Letter, we study a commensurate two-component bosonic system described by the on-site Hubbard Hamiltonian:

$$H = -\sum_{\langle ij\rangle\,\sigma}(t_\sigma a^\dagger_{i\sigma}a_{j\sigma} + \text{H.c.}) + \frac{1}{2}\sum_{i\,\sigma\sigma'} U_{\sigma\sigma'} n_{i\sigma} n_{i\sigma'}. \quad (1)$$

Here $a^\dagger_{i\sigma}$ creates a boson of the sort $\sigma = A, B$ on site i, $n_{i\sigma} = a^\dagger_{i\sigma}a_{i\sigma}$, and $\langle ij\rangle$ denotes pairs of nearest-neighbor sites. In what follows, we consider only equal filling factors of the components, $n_A = n_B = n$, with n integer, and, for brevity, denote $U_{AB} = -V$, $U_{\sigma\sigma} = U_\sigma$. A similar (incommensurate) two-species *bosonic* model has been studied recently to look at the differences with the *fermionic* Hubbard model [11].

At double commensurate filling, recent mean-field analysis of the model (1) in [12] failed to reveal phases and, correspondingly, phase transitions which cannot be reduced to simple mixtures of single-component states. This conclusion is disappointing considering predictions of other strongly correlated superfluid ground states for two-component inconvertible bosons: a paired superfluid vacuum (PSF), which is equivalent to the superfluid state of diatomic molecules and to a BCS superconductor [6,7,9,13]; and a super-counter-fluid (SCF), in which the net atomic superfluid current is zero, and yet the equal currents of the components in opposite directions are superfluid [8,13].

In this Letter, we perform Monte Carlo (MC) simulations of the $(d+1)$-dimensional classical analog of the on-site Hubbard model (1) and find five stable superfluid and insulating phases: (i) MI, (ii) MI of sort A and SF of sort B ($\text{MI}_\text{B}+\text{SF}_\text{A}$) and its A $\leftrightarrow$ B analog, (iii) SF of sort A and SF of sort B (2SF), (iv) PSF, and (v) SCF. An interacting mixture of two mutually penetrable superfluids (2SF) exists even without the optical lattice and corresponds to the $t \gg U_{\sigma,\sigma'}$ limit. This state has two nonzero complex order parameters $\langle\psi_A\rangle$ and $\langle\psi_B\rangle$. By increasing either U_B or U_A one drives the corresponding component from the superfluid to the Mott-insulating state; accordingly, in $\text{MI}_\text{B}+\text{SF}_\text{A}$ we have finite $\langle\psi_A\rangle$, and zero $\langle\psi_B\rangle$. When both U_A and U_B are strong, the ground state is MI with all order parameters being zero. Our proof then concerns the existence of PSF and SCF phases; in both phases $\langle\psi_A\rangle = \langle\psi_B\rangle = 0$, while $\Phi_\text{PSF} = \langle\psi_A\psi_B\rangle \neq 0$ in PSF, and $\Phi_\text{SCF} = \langle\psi_A\psi_B^\dagger\rangle \neq 0$ in SCF. It is worth noting that, while the PSF, representing atomic A + B pairing, requires $V > 0$, the SCF describes pairing of particles A and holes B and occurs when $V < 0$.

The most surprising MC result is that the 2SF-MI transition may be of I order. This result also follows from the mean-field (MF) analysis of the problem along the lines suggested in [3] for the single-component case. Finally, we develop microscopic arguments explaining why the I-order transition is generic for models with pairing interactions, and we show that MI ground states may be further classified in terms of their excitation spectrum.

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To prove that possible ground states of Eq. (1) include PSF, we assume the interexchange symmetry $A \leftrightarrow B$, implying $t_A = t_B = t$ and $U_A = U_B = U$ and consider the limit described by two strong inequalities: $t/U \ll 1$ and $\gamma/U \ll 1$, with $\gamma = U - V$ (here $V > 0$ and $\gamma > 0$; at $\gamma < 0$ the system collapses). Then, the effective low-energy Hilbert space is determined by states were on each site $n_{iA} = n_{iB}$; these are separated from other states by a large pair-breaking gap $\approx U$. We thus naturally arrive at the description in terms of *pairs*. In the second-order perturbation theory in t/U (cf., e.g., [8]) the dynamics of pairs is given by the effective Hamiltonian (we omit terms proportional to the total number of particles):

$$H_{\mathrm{p}} = -\tilde{t}\sum_{\langle ij\rangle}[(O_i^- O_j^+ + \mathrm{H.c.}) + 2m_i m_j] + \gamma\sum_i m_i^2. \quad (2)$$

Here m_i are pair occupation numbers, the raising operator O_i^+ is defined by $\langle m_i'|O_i^+|m_i\rangle = (m_i + 1)\delta_{m_i', m_i+1}$, $O_i^- = (O_i^+)^\dagger$, and $\tilde{t} = 2t^2/U$. In contrast to the standard single-boson hopping that scales linearly with the typical occupation number the hopping amplitude for pairs is quadratic in m_i. If potential energy terms in Eq. (2) were omitted, the ground state would collapse to a droplet with the diameter comparable to the lattice constant. The second term in the brackets, Eq. (2), describes nearest-neighbor attraction and further enhances collapse instability. A stable ground state arises only when the on-site repulsion γ is strong enough. On the other hand, at very large γ the commensurate ground state is MI. The question is then whether for some $\tilde{t}/\gamma$, the ground state is PSF rather than MI or collapsed. The positive answer is readily seen in the limit of a very large molecular filling factor $m = n/2 \gg 1$. In the region $\tilde{t} \ll \gamma \ll m^2\tilde{t}$ the system is stable against collapse; the nearest-neighbor attraction is negligible. Since the maximum insulating gap $\sim\gamma$ does not depend on m [4], we conclude that for $\gamma < m^2\tilde{t}$ the ground state must be superfluid. (Using mapping to the quantum rotor model [3] we know, in fact, that the MI state requires $\gamma > m^2\tilde{t}$.) Finally, for $m = 1$ we have performed quantum MC simulations of Eq. (2) in $d = 2$ and found that at $\gamma = 10\tilde{t}$ the ground state is superfluid.

Similarly, the existence of the SCF phase can be shown in the limit $t/U \ll 1$ and $|\tilde{\gamma}|/U \ll 1$ (where $\tilde{\gamma} = U + V$ and V is negative) studied in Ref. [8]. The effective Hamiltonian can be now written in terms of the spin-$S = (n_A + n_B)/2$ operators, $H_{\mathrm{S}} = -\tilde{t}\sum_{\langle ij\rangle}\mathbf{S}_i\mathbf{S}_j + \tilde{\gamma}\sum_i(S_{iz})^2$, which for small positive $\tilde{\gamma}$ has the easy-plane ferromagnetic ground state, or SCF [8]. Furthermore, one can show that PSF and SCF are qualitatively similar and SCF may be viewed as the result of pairing between particles of one component and holes of another [13]. *Because of this equivalence, we discuss below only the $V > 0$ case, that is, the case of the PSF.*

To reveal the global structure of the phase diagram we performed Monte Carlo simulations for the $(d + 1)$-dimensional classical analog of the bosonic Hubbard model. The so-called J-current model [14] is built on particle world lines (space-time currents) in discrete imaginary time, and we straightforwardly generalize it to the two-component case:

$$S = \sum_{\sigma,\sigma'}\sum_i \tilde{U}_{\sigma\sigma'}\,\vec{J}_i^{(\sigma)}\cdot\vec{J}_i^{(\sigma')}. \quad (3)$$

Here $\vec{J}_i^{(\sigma)}$ are integer-value currents [$(d + 1)$-dimensional vectors] subject to the local zero-divergence constraint, $\nabla\cdot\vec{J}_i^{(\sigma)} = 0$, and $\tilde{U}_{\sigma\sigma'} \sim U_{\sigma\sigma'}/t$ relates the effective action parameters to the original Hubbard Hamiltonian. This model has the same superfluid and insulating phases as Eq. (1), and we use it to understand the topology of phase boundaries, the existence of multicritical points, and first-order lines. We find it convenient to fix U_A and U_B and to plot results in the (V, ν) plane, where $\nu \sim 1/t$ is the scaling factor for all three dimensionless parameters. The superfluid phases are identified by looking at various superfluid stiffnesses, $\rho_s^{(\sigma)} = \langle[\vec{W}^{(\sigma)}]^2\rangle/dL^{d-2}$, $\rho_s^{(\mathrm{PSF/SCF})} = \langle[\vec{W}^{(A)} \pm \vec{W}^{(B)}]^2\rangle/DL^{D-2}$, expressed in terms of the winding number fluctuations [15], where $\vec{W}^{(\sigma)} = L^{-1}\sum_i\vec{J}_i^{(\sigma)}$ (superfluid stiffness and compressibility are equal in the space-time symmetric model).

In Fig. 1, we present the phase diagram of the two-component J-current model in $(d + 1 = 3)$ dimensions. Corresponding superfluid stiffness goes to zero continuously when approaching the lines of the critical points labeled as U(1). The correlation radius exponent (obtained from finite-size corrections) is consistent with the known value for the U(1) universality class in 3D. The first-order transition was identified by (i) a double-peak structure of the energy distribution function (in small-size systems) and (ii) hysteresis loops in all quantities (in large-size systems). Though we have not performed an exhaustive MC study of the phase diagram in other dimensions we found (i) the I-order 2SF-MI transition in $d = 3$ and (ii) no evidence for the first-order 2SF-MI transition in $d = 1$.

The I-order 2SF-MI line in the symmetric case ($U_A = U_B$) becomes strongly suppressed by the anisotropy, $U_A - U_B \neq 0$, between the components. For $U_B/U_A = 2$, the point where all four phases meet is already a simple cross of two U(1) lines—decoupled U(1) $\times$ U(1) tetracritical point (see, e.g., [16]). Points where the I-order line starts and ends represent multicritical points.

Normally, first-order transitions can be qualitatively accounted for in simple mean-field models, and we propose such a model for our case. Away from the multicritical region, all transitions are of the U(1)-universality class and, thus, described by the corresponding $|\psi|^4$ actions [4] for atomic, ψ_A, ψ_B, and molecular, Φ, fields. We arrive at the simplest effective free energy by combining three $|\psi|^4$ actions and writing the interaction term in the form of the molecule "creation/annihilation" process out of A and B particles. Omitting gradient terms,

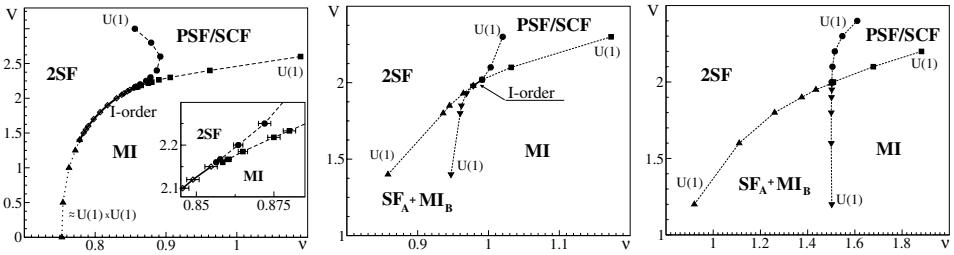

FIG. 1. Phase diagrams of the $d = 2$ two-component J-current model in the (V, ν)-plain for the symmetric, $U_A = U_B = 2$ (left), slightly asymmetric, $U_A = 1.6$, $U_B = 2$ (center), and strongly asymmetric, $U_A = 1$, $U_B = 2$ (right) models. The first-order phase transition line is dramatically reduced in the presence of weak anisotropy, and completely disappears for strong anisotropy between the components. All horizontal error bars are smaller than point sizes (typically of order 10^{-3}), and lines are used to guide the eye and to distinguish between different phase boundaries. The inset shows more clearly the region where 2SF, PSF, and MI phases meet. (Commensurability and intrinsic symmetry of the J-current model result in a straightforward mapping of the SCF regime onto PSF one: $V \to -V$.)

$$\mathcal{F} = \tfrac{1}{2}[r_A|\psi_A|^2 + r_B|\psi_B|^2 + r_M|\Phi|^2] + \tfrac{1}{4}[g_A|\psi_A|^4 + g_B|\psi_B|^4 + g_M|\Phi|^4] - g(\Phi^*\psi_A\psi_B + \text{c.c.}). \quad (4)$$

The mean-field phase diagram follows from minimization of $\mathcal{F}$. In Fig. 2, taking advantage of the scaling freedom for all the fields and $\mathcal{F}$, we set $g_a = g_B = g_M = g = 1$. It reproduces correctly the topology of boundaries between the phases and some of their properties. If the A-B asymmetry is not large, it features an I-order line; see Fig. 2. In the strongly anisotropic case, $|r_B - r_A| > 1$, the MF theory also captures the disappearance of the I-order transition. On another hand, the prediction of the pronounced I-order 2SF-PSF line does not agree with the numerical data in 3D. With our system sizes up to 128^3 sites we did not find any evidence for the I-order 2SF-PSF or 2SF-($\mathrm{MI_B}+\mathrm{SF_A}$) transitions; see the inset in Fig. 1. It is probably too early to draw the final conclusion on the structure of the multicritical point, because a similar study in 4D (for the system size 32^4) revealed a tiny (but finite) I-order 2SF-PSF line. In any case, the suppression of the I-order 2SF-PSF transition constitutes a strong deviation from the MF prediction.

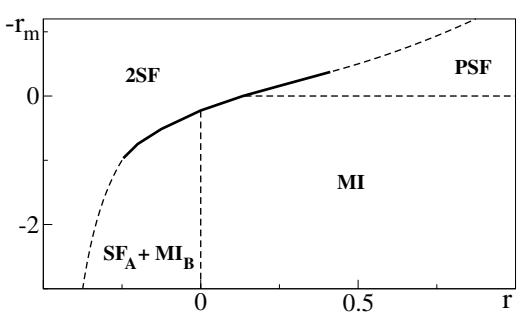

FIG. 2. The mean-field diagram for $r_A = r$, $r_B = r + 0.5$ The bold solid line corresponds to the first-order transition, and dashed lines describe continuous transitions. In the limit of $r_B \to r_A$, the $\mathrm{SF_A}+\mathrm{MI_B}$ domain vanishes.

First-order SF-MI transition in the single-component system.—It is generally accepted that in the single-component, commensurate Bose system the SF-MI transition is continuous [4]. Numerous simulations of the on-site Hubbard and J-current models perfectly agree with this picture (for the latest simulation, see [17]).

Excitations in MI are gapped and described as quasiparticles and quasiholes with the relativistic dispersion law at small momenta (for small gaps): $\epsilon(\mathbf{k}) = \sqrt{\Delta^2 + c^2k^2}$, where c is the velocity of sound in the SF phase. The dilute gas of quasiparticles is characterized by the effective mass $m_* = \Delta/c^2$ and some s-wave scattering amplitude, a_* (to be specific, we assume that $d = 3$). If the scattering length is positive, the state of the dilute excitation gas with density n_{qp} is stable, and the energy density cost of creating it is $E_{\mathrm{qp}} = (\Delta - \mu)n_{\mathrm{qp}} + (2\pi a_*/m_*)n_{\mathrm{qp}}^2$, where μ is the chemical potential. Since the effective long wave action for the U(1)-transition has a *positive* coefficient in front of the $|\psi|^4$ term, in the vicinity of the critical point the MI state is always described by positive a_*. As the chemical potential is increased above the threshold value Δ, the system state becomes superfluid (this continuous MI-SF transition, induced by adding extra particles/holes, is mean-field-like [4]).

Imagine now a MI state with gapped quasiparticle excitations, but now with *negative* effective scattering length. Although the MI vacuum itself may remain stable, the state of the quasiparticle gas at any small density $n_{\mathrm{qp}}|a_*|^3 \ll 1$ is unstable against collapse to a dense droplet. We thus conclude that this MI will undergo a first-order phase transition to the superfluid state at some $\mu = \mu_c$ finite distance below Δ to gain negative potential energy. Furthermore, if for some system parameters $\Delta \neq 0$, but $\mu_c = 0$, the MI-SF transition in the commensurate system will happen by the I-order scenario, too.

We now argue that MI states with negative a_* naturally arise in models with strong pairing interactions when potential energy favors two bosons on the same site, but increases fast for occupation numbers $n_i > 2$ to prevent

collapse. For sufficiently strong pairing, one may have a superfluid state of tight molecules, or PSF (cf. [18]). When repulsion between molecules is increased, PSF undergoes a standard continuous PSF-MI transition. In the vicinity of the transition point the lowest excitations above MI are *bound* bosonic pairs. We observe then, that depending on the value of the pairing interaction, there should exist at least three MI ground states distinguished by the value of the effective scattering length of its quasiparticles: as we go along line C in Fig. 3, a_* starts from a positive value (the quasiparticle gas is stable), then changes sign and becomes negative (the quasiparticle gas is unstable against collapse), and finally goes through the pole and changes sign again (the quasiparticle gas of molecules is stable). It seems unlikely that SF, PSF, and three different MI phases meet at the same point. In our view, the intersection of the SF-MI and $|a_*| = 0$ lines marks the beginning of the first-order SF-MI transition, while the intersection of the PSF-MI and $|a_*| = \infty$ lines marks its end. In this picture, the critical point where the SF-MI line changes from continuous to first order is characterized by the continuous Lorentz-invariant action with zero $|\psi|^4$ term.

In $d = 2$, the weak logarithmic dependence of a_* on quasiparticle density does not change the qualitative picture, because the first-order transition involves finite particle density jumps. In $d = 1$, the notion of the scattering length is ill-defined, and two quasiparticles in the long wave limit either form a bound state or repel each other like hard-core spheres. We conjecture then that in $d = 1$ (i) MI with first-order transition in μ does not exist and (ii) the SF-MI transition is always continuous.

The above considerations readily generalize to the A-B symmetric two-component case. Now, the criterion for the MI ground state, which is unstable against light doping by A and B particles (for the symmetric case $\Delta_A = \Delta_B = \Delta$), follows from the scattering matrix $(a_*)_{\sigma\sigma'}$ becoming nonpositive definite due to an increasing attraction between the components. We note that this criterion *must* be satisfied in a finite region in parameter space since the existence of AB molecules implies that $(a_*)_{AB}$ can be arbitrarily large and negative before going through the pole corresponding to the formation of the bound state. This consideration, in complete analogy with the single-component case, suggests that PSF-MI and 2SF-MI lines are "bridged" by the first-order line in agreement with MC simulations and MF analysis.

To explain the suppression and disappearance of the first-order region when the symmetry between the A and B components is broken (see Fig. 1) we suggest that, for strong anisotropy, the lowest excitations above the MI ground state in the whole parameter range are either A particles or AB molecules, and there is no reason for collective instability in the quasiparticle gas. Formally, this corresponds to pushing the $|(a_*)_{AB}| = \infty$ line into the

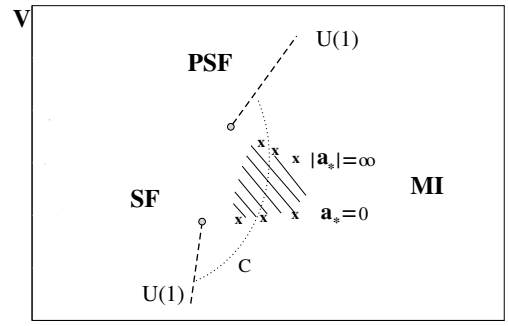

FIG. 3. Sketch of possible MI phases in the commensurate, n = even, single-component Hubbard model with pairing interactions and phase transition lines from MI to the SF and PSF phases. The region between the crosses is characterized by first-order MI-SF transition as a function of μ.

$SF_A + MI_B$ phase — this possibility does not exist in the symmetric case.

We are grateful to A. Patashinskii and S. Sachdev for fruitful discussions and valuable comments. This work was supported by the National Science Foundation and PSC CUNY grants. B. S. acknowledges also support from the Netherlands Organization for Scientific Research (NWO).

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