Bose-Einstein Condensation of Particle-Hole Pairs in Ultracold Fermionic Atoms Trapped within Optical Lattices

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We investigate the Bose-Einstein condensation (BEC, superfluidity) of particle-hole pairs in ultracold fermionic atoms with repulsive interactions and arbitrary polarization, which are trapped within optical lattices. In the strongly repulsive limit, the dynamics of particle-hole pairs can be described by a hard-core Bose-Hubbard model. The insulator-superfluid and charge-density-wave- (CDW) superfluid phase transitions can be induced by decreasing and increasing the potential depths with controlling the trapping laser intensity, respectively. The parameter and polarization dependence of the critical temperatures for the ordered states (BEC and/or CDW) are discussed simultaneously.

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In recent years, the demonstration of Bose-Einstein condensation (BEC) of particle-particle pairs in homogeneous or confined two-component (spin-1/2) fermionic atoms has triggered great theoretical and experimental interest. The BCS-BEC crossover in ultracold Fermi atomic gases near a Feshbach resonance has been predicted [1], and been observed [2]. For the fermionic atoms trapped within optical lattices, the s-wave or d-wave particle-particle pairs can undergo a phase transition to a superfluid state when the interaction is attractive or repulsive [3].

With the mechanism of superfluidity of atom-atom pairs in ultracold Fermi atomic gases being explored more and more deeply, a question arises as to whether the atom-hole pairs can undergo a BEC phase transition similar to electron-hole pairs [4]. First, because of the nonequilibrium nature of the system of particle-hole pairs, it becomes an ideal system for exploring the nonequilibrium quantum mechanics at the frontier of many-body physics. Additionally, since all condensed particle-hole pairs can emit photons in tandem, the quantum coherence in such a condensate reveals novel optical effects and nonlinear optical dynamics. This provides possible applications in ultrafast digital logical elements and quantum computation. Furthermore, the controllable interaction strength and kinetic energy in the atomic systems open up the very exciting potential to investigate macroscopic quantum coherence and superfluidity under some extreme conditions that never exist in electronic systems.

In this Letter, we show that the atom-hole pairs in arbitrarily polarized spin-1/2 ultracold Fermi atoms with repulsive interaction, which are trapped within optical lattices, can undergo a superfluid phase transition similar to the ultracold bosonic atoms [5]. In the strongly repulsive limit, the dynamics of atom-hole pairs obey a hard-core Bose-Hubbard model. The phase transition is analyzed with the derived Bose-Hubbard model. The critical temperature for the ordered states is discussed within the mean-field theory.

Consider an ensemble of polarized ultracold fermionic atoms occupying two different states $|S\rangle$ and $|P\rangle$, which are trapped within the optical lattices. For simplicity, we assume the optical lattice potentials as $V_0^{s,p}(\vec{x}) = \sum_{j=1}^{d} V_0^{s,p}\cos^2(kx_j)$. The wave vector k is determined by the laser wavelengths, d (= 1, 2, or 3) is the dimension, and $V_0^{s,p}$ are proportional to the laser intensity. For sufficient low temperature, the system obeys an asymmetric Fermi-Hubbard Hamiltonian [3]

$$H = -\sum_{\langle i,j\rangle}(t_s f_{si}^{+} f_{sj} + t_p f_{pi}^{+} f_{pj}) + \sum_i (\epsilon_s n_{si} + \epsilon_p n_{pi}) + U\sum_i n_{si} n_{pi}. \quad (1)$$

Here $f_{\sigma i}^{+}$ ($f_{\sigma i}$) are fermionic creation (annihilation) operators for atoms in state $|\sigma\rangle$ on site i, $n_{\sigma i} = f_{\sigma i}^{+} f_{\sigma i}$. The symbol $\langle i, j\rangle$ represents summing over the nearest neighbors, and ϵ_s (ϵ_p) is the single-atom energy of the atoms in state $|S\rangle$ ($|P\rangle$). The state-dependent tunneling t_s (t_p) can be induced by varying the potential depth V_0^s (V_0^p) [6]. Usually, the tunneling strengths increase with the decrease of potential depths. Below the unitary limit, U is proportional to the s-wave scattering length between atoms occupying different states. The s-wave scattering between atoms occupying the same state is absent due to the Pauli blocking.

The average number of atoms per site n and the polarization γ of the considered system are defined as

$$n = \sum_i (n_{si} + n_{pi})/N_L, \qquad \gamma = \sum_i (n_{si} - n_{pi})/N_T. \quad (2)$$

The symbol N_L is the total number of lattice sites, and $N_T = \sum_i (n_{si} + n_{pi})$. In the following, we focus our interests on the half-filled case ($n = 1$).

The ground state energy per atom depends upon both the polarization and the energy difference ($\Delta\epsilon = \epsilon_p - \epsilon_s$)

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between two occupied states. With the definition of polarization, the ground states can be divided into five different regimes: nonpolarized (NP) ground states with $\gamma = 0$, partially polarized in state $|S\rangle$ (PPS) with $0 < \gamma < 1$, partially polarized in state $|P\rangle$ (PPP) with $-1 < \gamma < 0$, fully polarized in state $|S\rangle$ (FPS) with $\gamma = 1$, and fully polarized in state $|P\rangle$ (FPP) with $\gamma = -1$. For the one-dimensional lattices ($d = 1$) with state-independent hopping ($t_s = t_p = t$), these regimes can be exactly obtained with the Bethe-ansatz [7]. The $\Delta\epsilon$ has two critical values

$$\Delta\epsilon_1^c = \begin{cases} \frac{|U|}{2} - 2t + \int_0^\infty \frac{4tJ_1(w)dw}{w[1+\exp(\frac{|U|w}{2t})]} & \text{for } U < 0, \\ 0 & \text{for } U > 0, \end{cases} \quad (3)$$

and

$$\Delta\epsilon_2^c = \begin{cases} 2t + |U| & \text{for } U < 0, \\ \sqrt{\frac{U^2}{4} + 4t^2} - \frac{U}{2} & \text{for } U > 0, \end{cases} \quad (4)$$

corresponding to the boundaries between different regimes. Here, $J_1(w)$ is the first kind of Bessel function with first order. The nonpolarized, partially polarized, and fully polarized regimes satisfy $|\Delta\epsilon| \leq \Delta\epsilon_1^c$, $\Delta\epsilon_1^c < |\Delta\epsilon| < \Delta\epsilon_2^c$, and $|\Delta\epsilon| \geq \Delta\epsilon_2^c$, respectively (see Fig. 1).

In the strongly repulsive limit ($0 < t_{s,p} \ll U$), the Fermi-Hubbard model is equivalent to an effective spin-1/2 Heisenberg model [8]. For the case of infinitely repulsive limit ($U/t_{s,p} \to +\infty$), the ground states (lowest energy states) have only one atom for each site, and their charge degrees of freedom are frozen. Under the strongly repulsive condition, $U/t_{s,p} \gg 1$, one can introduce the bosonic operators

$$b_j^+ \Leftrightarrow f_{sj}^+ f_{pj}, \qquad b_j \Leftrightarrow f_{pj}^+ f_{sj}, \\ n_j = b_j^+ b_j \Leftrightarrow \tfrac{1}{2} + \tfrac{1}{2}(n_{sj} - n_{pj}), \quad (5)$$

for the atom-hole pairs on site j. The operator b_j^+ (b_j) creates (annihilates) a pair of S atom (atom in $|S\rangle$) and P hole (hole in $|P\rangle$) on site j. These operators with different

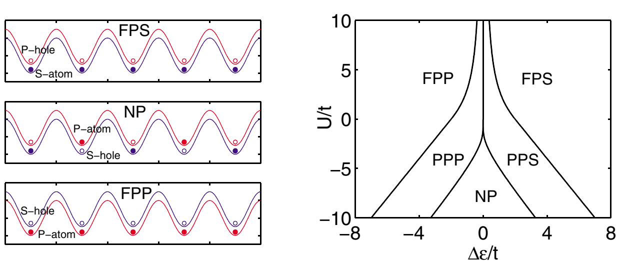

FIG. 1 (color online). Left: Ultracold fermionic atoms in one-dimensional optical lattices with half-filling and state-independent hopping. The dots and circles denote the atoms and holes (no atoms), respectively. Right: Polarization regimes of the ground states for the one-dimensional lattices with state-independent hopping.

lattice indices are commutable. However, to exclude the multiple occupation at each lattice that comes from Pauli blocking, the operators with the same lattice indices have a property like Fermi particles. In other words, the interaction between bosons on the same lattice is infinitely repulsive. Using the perturbation theory developed by Takahashi [8] (b and b^+ correspond to σ^- and σ^+), up to third order terms of the perturbation parameters (hopping strengths), we obtain the atom-hole pairs that obey the hard-core Bose-Hubbard Hamiltonian

$$H_B = -\mu \sum_i n_i + J \sum_{\langle i,j\rangle} b_i^+ b_j + V \sum_{\langle i,j\rangle} n_i n_j. \quad (6)$$

Denoting $t_p = \alpha t_s = \alpha t$, we obtain the hopping strength $J = 4t_p t_s/U = 4\alpha t^2/U$, the nearest-neighbor interaction strength $V = 2(t_s^2 + t_p^2)/U = 2(1 + \alpha^2)t^2/U$, and the chemical potential $\mu = \Delta\epsilon + ZV/2 = \Delta\epsilon + Z(1 + \alpha^2)t^2/U$. For the cubic lattices, the total number of the nearest neighbors Z equals $2d$. The above hard-core Bose-Hubbard model can be mapped onto an anisotropic spin-1/2 XXZ Heisenberg model with $J_{xy} = J$, $J_z = V$ and an effective magnetic field $B_z = \Delta\epsilon$ [9]. The antiferromagnetic-Z order, XY order, and fully magnetized states in the XXZ model correspond to the charge-density-wave (CDW) phase, superfluid phase, and fully polarized insulator phase of the atom-hole pairs, respectively [9,10]. The superfluidity means the Bose condensation of atom-hole pairs in their momentum spaces.

At zero temperature, the ground states for the atom-hole pairs have three different phases: (i) The charge-density-wave phase similar to a solid phase with zero polarization ($\gamma = 0$) corresponds to the half-filled case of the hard-core Bose-Hubbard model ($\langle b^+ b\rangle = 1/2$), (ii) the Bose-Einstein condensation phase corresponds with the nonzero superfluid order parameter $\langle b\rangle$, and (iii) insulator phase with the largest polarization ($|\gamma| = 1$) corresponds to the empty ($\langle b^+ b\rangle = 0$) or the fully filled ($\langle b^+ b\rangle = 1$) case of the hard-core Bose-Hubbard model. The difference between superfluid and insulator phases indicates that it needs a nonfully polarized atomic gas to support the atom-hole BEC. From the equivalence of the hard-core Bose-Hubbard model and the spin-1/2 XXZ Heisenberg model, using the path-integral method [11], one can obtain that the fully polarized insulator phase appears when $|\Delta\epsilon|/U > Z(t/U)^2(1 + \alpha)^2$, the BEC phase exists if $(Z/2)(t/U)^2\sqrt{(1 - \alpha^2)^2} < |\Delta\epsilon|/U < Z(t/U)^2 \times (1 + \alpha)^2$, and the CDW phase emerges when $|\Delta\epsilon|/U < (Z/2)(t/U)^2\sqrt{(1 - \alpha^2)^2}$. The separatrix between the CDW phase and the BEC phase corresponds to a first order phase transition. The points on this separatrix show the coexistence of both phases; they represent the supersolid phase. These conditions also show that the CDW-superfluid and insulator-superfluid transitions occur at $|\Delta\epsilon|/U = (Z/2)(t/U)^2\sqrt{(1-\alpha^2)^2}$ and $|\Delta\epsilon|/U = Z(t/U)^2(1+\alpha)^2$, respectively.

In Fig. 2, we show the phase diagram for lattices of arbitrary dimensionality with hopping ratio $\alpha = 2$. For fixed values of hopping ratio α, energy difference $\Delta\epsilon$, and on-site repulsive interaction strength U, increasing (decreasing) the hopping strength t induces an insulator-superfluid (solid-superfluid) transition. This means that Bose condensation of the atom-hole pairs exists for mediate hopping strengths. For larger (smaller) hopping strength, the ground states fall into the phase of CDW (fully polarized insulator). In the case of state-independent hopping, $\alpha = 1$, the CDW region becomes a line localized at $\Delta\epsilon = 0$. This is consistent with the results of the antiferromagnetic phase in Refs. [3].

At finite temperatures, due to the thermal fluctuations, the ordered phases are destroyed when the temperature is above some critical temperatures. Within the framework of the mean-field theory [12], a continuous phase transition between the CDW and the normal liquid (NL) takes place at the critical temperature

$$T^C_{\mathrm{CDW}} = \frac{Z}{k_B}\frac{(1+\alpha^2)t^2}{U}(1-\gamma^2), \quad (7)$$

and a similar phase transition between the superfluid and the normal liquid occurs at

$$T^C_{SF} = \frac{Z}{k_B}\frac{2\alpha t^2}{U}\frac{\gamma}{\mathrm{arctanh}(\gamma)}. \quad (8)$$

Here, k_B is the Boltzmann constant. The bicritical polarizations $\gamma = \pm\gamma^{BC}(\alpha)$ $(\gamma^{BC} > 0)$ are given by $T^C_{SF} = T^C_{\mathrm{CDW}}$ and $|\gamma| \neq 1$. Below the critical temperatures, there are two coexistence regions of CDW and superfluid, which correspond to the supersolid regions. The boundaries between the superfluid and the supersolid and between the CDW and the supersolid can be obtained by using the Landau expansion [13]. At zero temperature, the critical polarization corresponding to the superfluid-supersolid transition is given as $\gamma^{SFC} = |(1-\alpha)/(1+\alpha)|$. For the case of state-independent hopping ($\alpha = 1$), the critical polarization $\gamma^{SFC} = 0$, it means that the CDW-solid and supersolid regions shrink to a line localized at $\gamma = 0$. This indicates that the atom-hole BEC in nonpolarized atoms with state-independent hopping has the highest critical temperature for the superfluid phase.

The finite-temperature phase transitions rely on the hopping ratio α and the polarization γ. For state-independent hopping ($\alpha = 1$), CDW-NL and superfluid-NL transitions occur in nonpolarized ($\gamma = 0$) and polarized ($\gamma \neq 0$) cases, respectively. For state-dependent hopping ($\alpha \neq 1$), the transition routes become more complex. The CDW-NL, supersolid-CDW-NL, superfluid-supersolid-CDW-NL, and superfluid-NL phase transitions take place when $\gamma = 0$, $0 < |\gamma| \leq \gamma^{SFC}$, $\gamma^{SFC} < |\gamma| < \gamma^{BC}$, and $|\gamma| \geq \gamma^{BC}$, respectively.

The critical temperatures are determined by both the parameters and the polarization. The parameter dependence is similar to the one of Refs. [3], $T^C \propto t^2/U$. Thus, to increase the critical temperatures, one has to decrease the potential depths $V_0^{s,p}$ to increase the hopping strengths. The polarization dependence of the critical temperatures and the finite-temperature phase diagram are shown in Fig. 3 for the state-dependent hopping case with $\alpha = 2$.

The previous consideration includes only the terms up to the third order of the perturbation parameter. Including up to the fifth order terms, the Hamiltonian (6) reads as

$$H_B = -\mu\sum_i n_i + J_1\sum_{\langle i,j\rangle} b_i^+ b_j + J_2\sum_{\langle\langle i,k\rangle\rangle} b_i^+ b_k + V_1\sum_{\langle i,j\rangle} n_i n_j + V_2\sum_{\langle\langle i,k\rangle\rangle} n_i n_k. \quad (9)$$

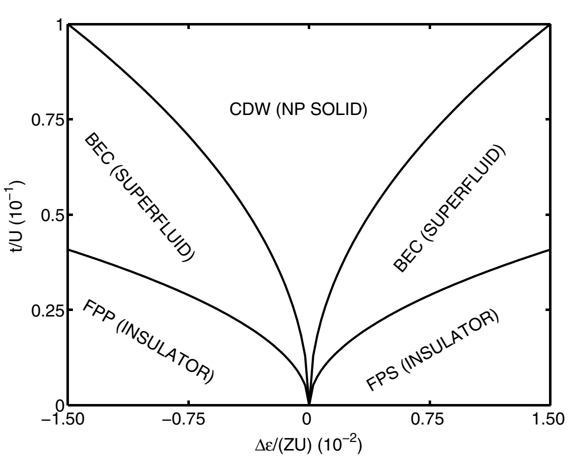

FIG. 2. Zero-temperature phase diagram of the ground states for the atom holes in arbitrarily dimensional lattices with $\alpha = 2$.

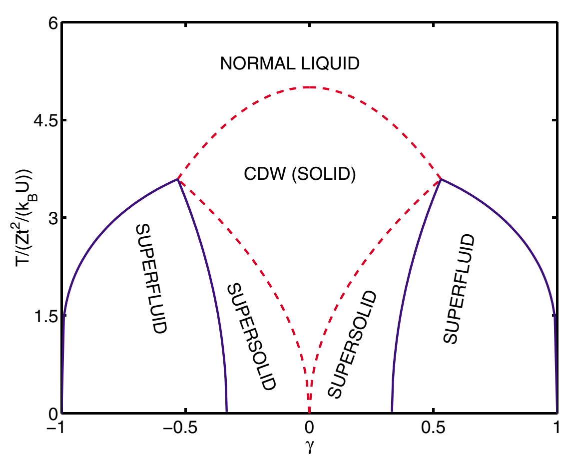

FIG. 3 (color online). Mean-field finite-temperature phase diagram for the atom-hole pairs in state-dependent hopping case with $\alpha = 2$.

Here, $\langle\langle i, k\rangle\rangle$ represents summing over the next-nearest neighbors. The parameters are determined by $\mu = \Delta\epsilon + Z(V_1 + V_2)/2$, $J_1 = \frac{4t_s t_p}{U}[1 - \frac{2(t_s^2+t_p^2)}{U^2}]$, $V_1 = \frac{4t_s t_p}{U} \times (\frac{t_s^2+t_p^2}{2t_s t_p} - \frac{t_s^4+t_p^4+6t_s^2t_p^2}{2U^2 t_s t_p})$, $J_2 = \frac{4t_s^2t_p^2}{U^3}$, and $V_2 = \frac{4t_s^2t_p^2}{U^3}(3t_s^4 + 3t_p^4 - 4t_s^2t_p^2)/(2t_s^2t_p^2)$. The corresponding critical temperatures are formulated as

$$T_{\rm CDW}^C = \frac{Z}{2k_B}(V_1 - V_2)(1 - \gamma^2), \tag{10}$$

$$T_{SF}^C = \frac{Z}{2k_B}(J_1 + J_2)\frac{\gamma}{\operatorname{arctanh}(\gamma)}. \tag{11}$$

Because $J_2 \ll J_1 \approx J$ and $V_2 \ll V_1 \approx V$, the above equations indicate that the critical temperatures are shifted only a little bit by the high-order terms.

In summary, we have demonstrated the existence of Bose-Einstein condensation of atom-hole pairs in arbitrarily polarized ultracold fermionic atoms confined in optical lattices with half-filling. In the strongly repulsive limit, the atom-hole pairs obey a hard-core Bose-Hubbard Hamiltonian. For a polarized insulator phase, the particle-hole pairs undergo an insulator-superfluid transition when the hopping between nearest neighbors is increased. For a CDW phase, the pairs undergo a CDW-superfluid transition when the hopping is decreased. The mean-field results indicate that the finite-temperature phase transition depends upon not only the system parameters but also the polarization.

To realize the model, one can prepare ultracold two-component atomic Fermi gases with arbitrary polarization [2], then load them into an optical lattice with one atom per site. The optical lattices can be produced with a series of standing-wave lasers. Similar to the realization of Tonks gas [14] (the physical details are only loosely related), the strongly repulsive limit $U/t_{s,p} \gg 1$ can be reached by increasing the s-wave scattering length with Feshbach resonances [15] (still below the unitary limit [16]) and/or by decreasing the hopping strengths $t_{s,p}$ with controlling the laser intensity. The applied magnetic field also induces an energy difference between two occupied levels due to the Zeeman effects. To observe the superfluidity, one can use the Bragg scattering approach to detect the elementary excitations spectrum of cold atoms [17]. In a condensed system of interacting atom-hole pairs within an applied electromagnetic field, the stimulated two-photon emission process can also give credible evidence for the atom-hole BEC [18].

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