Holon Pair Condensation and Phase Diagram of High $T_c$ Cuprates

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A possibility of holon (boson) pair condensation is explored for hole doped high $T_c$ cuprates, by using the U(1) slave-boson representation of the $t$-$J$ Hamiltonian with the inclusion of hole-hole repulsion. A phase diagram of the hole doped high $T_c$ cuprates is deduced by allowing both the holon pairing and spinon pairing. It is shown that the spin gap size remains nearly unchanged below the holon pair condensation temperature. We find that the $s$-wave holon pairing under the condition of $d$-wave singlet pairing is preferred, thus allowing $d$-wave hole pairing.

I. INTRODUCTION

It is believed that the high $T_c$ superconductivity arises as a result of Bose condensation of doped holes. It is still an unresolved problem to predict a satisfactory phase diagram of involving the Bose condensation of the doped holes and the normal state pseudogap. The normal state pseudogap has been observed in various experiments \[10\]: NMR \[11\], neutron scattering \[12\], c-axis optical conductivity \[13\], heat capacity \[14\], in-plane resistivity \[15\] and photoemission \[16\]. A universal dependence of conductivity \[4,5\], heat capacity \[6\], in-plane resistivity \[8\] optimal doping rate of $T_c$ pseudogap has been observed in various experiments beyond it. This observation is well fit by a universal relation, $T_c/T_c^{\text{max}} = 1 - 82.6(x - 0.16)^2$ where $T_c^{\text{max}}$ is the maximum critical temperature at the optimal doping rate of $x = 0.16$ \[1\].

Based on the $t$-$J$ model Hamiltonian, the normal state pseudogap is regarded as the spin gap \[12,13\]. Earlier superconductivity in the underdoped cuprates was understood as a simultaneous presence of the spin gap and single boson (holon) condensation \[11,15\]. Recently an SU(2) slave-boson theory of the $t$-$J$ model Hamiltonian was proposed to allow symmetry at both half filling and finite doping \[12,20\]. In this theory \[15\] single boson (holon) condensation can be either completely destroyed or reduced due to a low lying fluctuation (soft mode) in association with the SU(2) rotation, and thus boson (holon) pair condensation is suggested \[20\]. Earlier various preformed-pair scenarios \[21,23\] were proposed. In one of the scenarios \[23\], the preformed pairs become locally available below the pseudogap temperature, and the critical temperature of superconductivity is determined by phase ordering of the preformed pairs. On the other hand, numerical calculations \[24,27\] have been made to study the pairing of doped holes in the $t$-$J$ clusters and $t$-$J$ ladder systems. A recent study for doped $t$-$J$ three-leg ladders \[28\] revealed hole pairing due to the coupling of a Luttinger liquid to the insulating or doped spin liquid. In view of great interest in the role of doped holes for high $T_c$ superconductivity, we investigate a possibility of boson pair condensation by introducing a modified $t$-$J$ Hamiltonian and derive a phase diagram in the plane of temperature vs. hole doping rate.

II. MEAN FIELD HAMILTONIAN AND FREE ENERGY FROM A MODIFIED $t$-$J$ HAMILTONIAN IN THE SLAVE-BOSON REPRESENTATION

A necessity of introducing the electrostatic hole-hole repulsion is stressed in recent numerical studies of a spin ladder system \[27,29\]. In order to account for a reasonable hole pair binding a large value of Coulomb repulsion energy $V$ between two nearest neighbor (NN) holes was needed, i.e., $V = e^2/(\epsilon_\infty a_0) = 0.1 eV$ \[27\] with $a_0 \approx 3.8 A$, the lattice constant and $\epsilon_\infty = 30 \sim 40$, the dielectric constant \[30\]. Ignoring this repulsion energy, the bound state of the hole pairs was found to be excessively robust \[29\].

In the local U(1) symmetry conserving slave-boson representation, we write the full $t$-$J$ Hamiltonian of the two dimensional systems of antiferromagnetically correlated electrons by including a hole-hole repulsion term,

$$H = -t \sum_{\langle i,j \rangle} (f_{i\sigma}^\dagger b_i b_j f_{j\sigma} + \text{h.c.}) + J \sum_{\langle i,j \rangle} \left( S_i \cdot S_j - \frac{n_i n_j}{4} \right)$$

$$+ V \sum_{\langle i,j \rangle} b_i^\dagger b_i^\dagger b_j b_j - \mu_0 \sum_i f_{i\sigma}^\dagger f_{i\sigma} (1)$$

with $S_i = 1/2 f_{i\sigma}^\dagger \sigma_{\alpha\beta} f_{i\beta}$. Here the local constraint of single occupancy, $\sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} + b_i^\dagger b_i = 1$ is assumed. $f_{i\sigma}^\dagger (f_{i\sigma})$ is the spinon creation (annihilation) operator and $b_i(b_i^\dagger)$, the holon annihilation (creation) operator. The third term represents Coulomb repulsion between holes in the NN sites; according to an experiment \[11\] the hole-hole repulsion decays rapidly with distance. The second bracketed term above implies that the NN configuration of two holes is energetically more favorable than other possible configurations. This is because the two holes in the NN sites break 7 bonds compared to 8 bonds for other configurations. This is evident from the separate inspection of the two attractive interaction terms, $JS_i \cdot S_j$ and $-(J/4)n_i n_j$. For the latter we write,
\[-J \sum_{\langle i,j \rangle} \frac{n_i n_j}{4} = -\frac{J}{4} \sum_{\langle i,j \rangle} \left\{ 1 - b_i^\dagger b_i - b_j^\dagger b_j + b_i^\dagger b_j^\dagger b_i b_j \right\} \]
\[-\frac{J}{2} \sum_{i \sigma} f_{i \sigma} f_{i \sigma} + \frac{J}{2} \sum b_i^\dagger b_i = \frac{J}{4} \sum_{\langle i,j \rangle} b_i^\dagger b_i b_j. \]

where the local constraint of single occupancy is considered. The effective attraction between the NN holes arises from the last term of the equation above.

Applying the Hubbard-Stratonovich transformation

\[
H = \sum_{\langle i,j \rangle} \frac{3J}{8} |\chi_{ji}|^2 + |\Delta_{ji}^f|^2 - \left( \frac{8t}{3J} b_j^\dagger b_i + f_{j \sigma}^\dagger f_{i \sigma} \right) \chi_{ji} - h.c. - (f_{j \uparrow} f_{i \downarrow} - f_{j \downarrow} f_{i \uparrow}) \Delta_{ji}^f - h.c. \]
\[+ \frac{8t^2}{3J} \sum_{\langle i,j \rangle} (b_j^\dagger b_i) (b_i^\dagger b_j) - \sum_{\langle i,j \rangle} \left( \frac{J}{4} - V \right) b_i^\dagger b_i b_j - \left( \mu_0 - \frac{1}{4} \right) \sum_{i} f_{i \sigma}^\dagger f_{i \sigma} + \frac{J}{2} \sum b_i^\dagger b_i \]
\[\quad - i \sum \lambda_i (f_{i \sigma}^\dagger f_{i \sigma} + b_i^\dagger b_i - 1), \]

where a Lagrange multiplier field \(\lambda_i\) is introduced for the local constraint of single occupancy for both the spinon and the holon. The quartic holon term (the second term in Eq. (3) above), \(\frac{8t^2}{3J} \sum_{\langle i,j \rangle} (b_j^\dagger b_i) (b_i^\dagger b_j)\) is repulsive \(\text{(22)}\). It is important to realize that this term corresponds to the holon exchange interaction, but not to the direct (forward) interaction nor to the holon pairing interaction.

Thus allowing only the holon exchange channel, we linearize the quartic holon term (the second term in Eq. (3)) as

\[
\frac{8t^2}{3J} \sum_{\langle i,j \rangle} (b_j^\dagger b_i) (b_i^\dagger b_j) = \frac{8t^2}{3J} \sum_{\langle i,j \rangle} (\langle b_j^\dagger b_i \rangle b_i^\dagger b_j + b_i^\dagger b_i (b_i^\dagger b_j) - \langle b_j^\dagger b_i \rangle (b_i^\dagger b_j)). \]

We decompose the effective holon attractive energy term (the third term in Eq. (3)), that is, \(-\sum_{\langle i,j \rangle} \left( \frac{J}{4} - V \right) b_j^\dagger b_i^\dagger b_j b_i\) with \(0 < V < J/4\) into the direct, exchange, and pairing channels \(\text{(23)}\). By introducing the Hubbard-Stratonovich transformation for the resulting holon pairing term and the above linearized holon exchange term, we obtain

\[
H = \sum_{\langle i,j \rangle} \frac{3J}{8} |\chi_{ji}|^2 + |\Delta_{ji}^f|^2 - \left( \frac{8t}{3J} b_j^\dagger b_i + f_{j \sigma}^\dagger f_{i \sigma} \right) \chi_{ji} - h.c. - (f_{j \uparrow} f_{i \downarrow} - f_{j \downarrow} f_{i \uparrow}) \Delta_{ji}^f - h.c. \]
\[+ \sum_{\langle i,j \rangle} \left( \frac{J}{4} - V \right) \left[ |\Delta_{ji}^h|^2 - b_j^\dagger b_j \Delta_{ji}^h - h.c. \right] - \sum_{\langle i,j \rangle} \frac{8t^2}{3J} \left( \frac{J}{4} + V \right) \left[ \langle b_j^\dagger b_i \rangle (b_i^\dagger b_j) - b_j^\dagger b_i (b_i^\dagger b_j) - h.c. \right] \]
\[\quad - \mu_0^f \sum_{i} f_{i \sigma}^\dagger f_{i \sigma} - \mu_0^h \sum_i b_i^\dagger b_i - \sum \lambda_i (f_{i \sigma}^\dagger f_{i \sigma} + b_i^\dagger b_i - 1), \]

with \(\mu_0^f = \mu_0 - J/4\) and \(\mu_0^h = -3J/4\), where \(\Delta_{ji}^h\) is now the Hubbard-Stratonovich field for holon pairing. Here \(\mu_0^f\) and \(\mu_0^h\) are the effective chemical potentials for the spinon and the holon respectively. Obviously the two scalar fields, \(\chi_{ji} = \langle 8t/3J b_j^\dagger b_i + f_{j \sigma}^\dagger f_{i \sigma} \rangle\) and \(\langle b_j^\dagger b_i \rangle\) in Eq. (3) above are not independent. We allow a linear relation between the spinon hopping and the holon hopping order parameters, i.e., \(f \sum f_{j \sigma}^\dagger f_{i \sigma} = \eta \langle b_j^\dagger b_i \rangle\). Thus we rewrite \(\chi_{ji} = (8t/3J) + 2\eta \langle b_j^\dagger b_i \rangle\) and

\[
\langle b_j^\dagger b_i \rangle = \frac{1}{8t/(3J) + 2\eta} \chi_{ji}. \]

A self-consistent determination of the hopping ratio \(\eta\) will be discussed later.

Substitution of Eq. (4) into Eq. (3) results in the cancelation of terms (proportional to \(\frac{8t^2}{3J}\)) involving the holon exchange channel in Eq. (3). By defining the pairing order parameters \(\Delta^p_i = \langle f_{j \uparrow} f_{j \downarrow} - f_{j \downarrow} f_{j \uparrow} \rangle\) and \(\Delta^h = \langle b_j^\dagger b_j \rangle\) with \(\tau = \bar{x}\) or \(\bar{y}\), and allowing the uniform hopping order parameter, \(\chi_{ji} = \chi\), the resulting mean field Hamiltonian is
Now, consider the spinon hopping order field, that is, \( \Delta_{f}^2 - (f_{j\uparrow}f_{j+r,\downarrow} - f_{j\downarrow}f_{j+r,\uparrow})\Delta_{f}^* \) h.c. - wave spinon pairing with \( \Delta_{f} \) and \( \Delta_{f}^* \) respectively at various \( j \). For the present study, we determine the hopping ratio \( \eta \) self-consistently with the use of \( \sum_{\sigma}(f_{j\uparrow}f_{j\sigma}) = -\frac{1}{2N}\sum_{k}\left[\gamma_k(c_{k}\downarrow - \mu^f)/E_k\right] \tanh(\beta E_k/2) \) and \( \langle b_{j\uparrow}b_{j\uparrow}\rangle = \frac{1}{N}\sum_{k}\left[\gamma_k(c_{k}\downarrow - \mu^b)/E_k\right] \coth(\beta E_k/2) \).

III. COMPUTED RESULTS OF BOSON (HOLON) PAIR CONDENSATION AND SPIN GAP TEMPERATURES; PHASE DIAGRAM OF \( T-x \) PLANE

In Fig. 1 we show as a function of doping rate the predicted spin gap \( E_{g}'(\pi, 0) = \frac{4J}{\Delta_{f}} \) the rescaled hopping order parameter \( \frac{\Delta_{f}}{\Delta_{f}^\prime} \) \( \chi \) multiplied by \( \frac{\Delta_{f}}{\Delta_{f}^\prime} \), and the holon pairing order parameter \( \Delta_{b} \) respectively at various selected temperatures. The self-consistently determined result of \( \eta \) is found to be \( \eta \approx 0.2(1-x)/x \) with \( x > 0.01 \) for \( J = 0.4t \). For the present study, \( J = 0.4t \) and \( V = 0.24999J \) were chosen to best fit the experimental phase diagram in the plane of \( T \) vs. \( x \). The predicted spin gap \( E_{g}'(\pi, 0) \) (y-axis on the left hand side) at \( k = (\pi, 0) \) decreases with the hole doping rate \( x \) at all temperatures. We find that the minimum of the free energy occurs only with the s-wave holon pairing, but not with the d-wave holon pairing. The d-wave holon pairing is found to be unstable. In Fig. 1. the s-wave holon pairing order parameter \( \Delta_{b} \) (y-axis on the right hand side) is displayed at each selected finite temperature. It is seen to increase with \( x \) at all temperatures. We now examine...
FIG. 1. The computed spin gap $E_g^f$ (on the left axis) at $k = (\pi, 0)$, the hopping order parameter $x$ multiplied by $3J/4$ (on the left axis) and holon pairing order parameter $\Delta^b$ (on the right axis) at various selected temperatures.

the variation of the spin gap with temperature below and above the holon pair condensation temperature, $T_{b\text{MF}}$ in the underdoped region. As an example, let us choose the doping rate of $x = 0.1$, at which $T_{b\text{MF}}$ is obtained to be 0.028J. Two of the three nearly indistinguishable lines of the spin gap $E_g^f(\pi, 0)$ at $T = 10^{-10}$J and $T = 0.02J$ (both of which represent temperatures below $T_{b\text{MF}}$) indicate nearly identical spin gap sizes. Thus the spin gap size remains nearly unchanged below the holon pair condensation temperature. The remaining four lines which correspond to temperatures above $T_{b\text{MF}}$ show a consistent decrease in the spin gap size as temperature increases.

In Fig. 2, we present the computed phase diagram in the $T$ – $x$ plane. The holon (boson) pair condensation temperature $T_{b\text{MF}}$ and the spin gap temperature $T_{b\text{MF}}$ are plotted as a function of doping rate $x$, including the spin gap $E_g^f(\pi, 0)$ at $T = T_{b\text{MF}}$. The mean field holon pair condensation temperature is found to be less than 0.1J in the underdoped region. In this region both the $d$-wave spinon pairing with $\langle f_1^\uparrow f_{j1}^\downarrow \rangle \neq 0$ and the $s$-wave holon pairing with $\langle b_i b_j^\dagger \rangle \neq 0$ exist below the mean field (critical) temperature ($T_c = T_{b\text{MF}}$). For the holon (but not the holon) pairs, we have $\langle c_{1\uparrow} c_{j\downarrow} \rangle = \langle b_i b_j^\dagger \rangle \langle f_1^\uparrow f_{j1}^\downarrow \rangle \neq 0$ in the mean field approximation. For clarity we would like to stress that the term, ‘holon’ refers to the boson of spin 0 and the term, ‘hole’ is the fermion of spin up and spin down. Thus this allows for the condensation of the $d$-wave hole pairs by satisfying the $s$-wave holon pairing for $\langle b_i b_j^\dagger \rangle$ and the $d$-wave pairing for $\langle f_{1\uparrow} f_{j1}^\downarrow \rangle$ in $\langle c_{1\uparrow} c_{j\downarrow} \rangle = \langle b_i b_j^\dagger \rangle \langle f_1^\uparrow f_{j1}^\downarrow \rangle$. Thus $T_{b\text{MF}}$ at each doping rate corresponds to the mean field critical temperature of the $d$-wave superconducting phase transition.

The mean field spin gap (pseudogap) temperature $T_{b\text{MF}}$ may be regarded as the ‘center’ of crossover region which arises as a result of gauge fluctuations \[10\]. The predicted pseudogap (spin gap) temperature $T_{b\text{MF}}^f$ is seen to smoothly decrease with the hole doping rate as shown in Fig. 2. This is consistent with the recent experiments \[11\]. The spin gap $E_g^f(\pi, 0)$ at the s-wave holon pair ($d$-wave hole pair) condensation temperature $T_{b\text{MF}}$ is predicted to show a rapid decrease with $x$ as is shown in Fig. 2. This spin gap (pseudogap) vanishes at the critical doping rate of $x_{cr} \simeq 0.19$, at which $T_{b\text{MF}}$ approaches $T_{b\text{MF}}^f$. We find that the position of the critical doping rate is sensitive to the choice of $V$. Unlike $T_{b\text{MF}}^f$, $T_{b\text{MF}}^c$ is nearly independent of $V$. The critical doping rate $x_{cr}$ decreases as $V$ gets smaller. With the choice of a vanishingly small value of $V$, we find that the value of holon pair order parameter $\Delta^b$ (and thus $T_{b\text{MF}}$) is excessively large even at a small doping rate. This is consistent with a recent numerical study \[29\]. The choice of $V = 0.24999J$ fits the experimental value of the observed critical doping rate of $x_{cr} = 0.19$ \[10,10\]. For this case the effective NN attractive energy is about $V_{\text{eff}} = \frac{1}{2} - V \simeq 10^{-5}J$. Earlier the mean field single holon condensation temperature was reported to be $T_{BE} = 2\pi xc0^{-2}/mk \[17,18\]$. It is displayed in Fig. 2 for comparison with our computed boson pair condensation temperature ($T_c = T_{b\text{MF}}$). Obviously we find a wide difference between the two Bose condensation temperatures of the holon-pair boson and the single holon boson. The observed optimal doping rate of $x_{\text{opt}} = 0.16$ \[17\] is known to be smaller than the critical doping rate of 0.19 \[10,10\]. In disagreement with observations, our predicted boson pair (not single boson) condensation temperature above the critical doping rate of $x_{cr} = 0.19$ becomes larger than the pseudogap (spin gap) temperature. Earlier it was suggested that the
overdoped region may correspond to the region where the mean-field solution is not stable with respect to the gauge fluctuations \[ \text{and that the system can probably be described by the Fermi liquid theory \[16, 34\]. However, it remains to be seen for a rigorous verification in the future.}

In Fig. 3 we present the effective holon chemical potential \( \mu^b(T = 0) \) (on the right axis) and the inverse of the holon compressibility \( 1/\kappa_b \) (on the left axis) as a function of doping rate \( x \). The computed spinon chemical potential decreases monotonically with doping rate. On the other hand, the holon chemical potential decreases up to \( x \approx 0.07 \) and starts to increase beyond this value. Allowing that the inverse of two dimensional holon compressibility \( \kappa_b \) holds for \( 1/\kappa_b = \frac{N^2 \rho^b}{\kappa^3 A} = \frac{N^2 \rho^0}{2 \kappa^3} \) (where \( N \) is the number of bosons and \( A \) is the area), we find that \( 1/\kappa_b \) is negative below \( x \approx 0.07 \) and becomes positive for \( x > 0.07 \). This suggests that in the region of \( x < 0.07 \) the holon pair condensation is unstable \[10\] and it is stable only for \( x > 0.07 \). The shaded region in Fig. 2 represents the region at which the holon pair condensation is unstable. It is well known that the superconductivity arises for \( x > 0.05 \) \[11\]. Interestingly recent numerical studies \[20, 23\] of \( t-J \) three-leg ladders revealed that there exist a critical doping rate of \( x \approx 0.06 \) beyond which the hole pairing increases rapidly as hole density increases. It is of great interest to see in the future whether there exists any possible relevance between the present result with the prediction of the \( t-J \) three-leg ladders study.

IV. CONCLUSION

A possibility of boson (holon) pair condensation was described with the inclusion of a repulsive interaction between the NN holes in the \( t-J \) Hamiltonian. A phase diagram of the hole-doped high \( T_c \) cuprates is derived by considering both the holon pair condensation and the spinon pairing gap (spin gap). In the mean field approximation, we note that \( \langle c_{i\uparrow} c_{j\downarrow} \rangle = \langle b_i^\dag b_j^\dag \rangle \langle f_{i\uparrow} f_{j\downarrow} \rangle \) for the hole pair. To avoid confusion, we would like to point out that the term, ‘hole’ stands for the fermion of positive charge \(+e\) with spin \(1/2\), while the term, ‘holon’ refers to the boson of positive charge \(+e\) with spin \(0\). We find that the \( s\)-wave holon pairing \( \langle b_i^\dag b_j^\dag \rangle \) but not the \( d\)-wave holon pairing is stable for the \( d\)-wave spinon pairing \( \langle f_{i\uparrow} f_{j\downarrow} \rangle \), thus allowing the condensation of \( d\)-wave hole pairs in the language of ‘hole’. In addition, it is shown that the spin gap remains nearly unchanged below the holon pair condensation temperature.

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$$\hat{v}_E = -\frac{1}{4} (b_i^\dagger b_j)(b_j^\dagger b_i)$$
$$\hat{v}_P = -\frac{1}{4} (b_i^\dagger b_i)(b_j^\dagger b_j)$$
$$\hat{v}_D = +\frac{1}{4} (b_i^\dagger b_j)(b_j^\dagger b_i) = \frac{1}{4} n_i n_j,$$

where $n_i = b_i^\dagger b_i$ is holon number operator at site $i$.
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