Importance of Coupling between the Charge and Spin Degrees of Freedom in High $T_c$ Superconductivity

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Based on an improved SU(2) slave-boson approach showing coupling between the charge and spin degrees of freedom, we derive a phase diagram of high $T_c$ cuprates which displays both the superconducting and pseudogap phases in the plane of temperature vs. hole doping rate. It is shown that phase fluctuations in the order parameters results in a closer agreement with the observed phase diagram of an arch shape, by manifesting the presence of an optimal doping rate.

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High $T_c$ superconductivity arises as a consequence of hole(or electron) doping in the parent cuprate oxides which are Mott insulators with antiferromagnetic long-range order. The observed phase diagram in the plane of temperature $T$ vs. hole doping rate $\delta$ shows the Bose condensation(superconducting temperature) curve of an ‘arch’ shape rather than the often predicted linear increase, by manifesting the presence of the optimal doping rate of $\delta = 0.16$ to 0.2. On the other hand, the observed pseudogap temperature displays nearly a linear decrease with $\delta$. The high $T_c$ cuprate of $Bi_2Sr_2CaCu_2O_{8+\delta}$ with a higher pseudogap(spin gap) temperature $T^\ast$ is observed to have a higher superconducting transition temperature $T_c$ than the cuprate of $La_{2-x}Sr_xCuO_4$ with a lower $T^\ast$. Further we find from the observed phase diagrams of both cuprates above that the two different high $T_c$ cuprates, $La_{2-x}Sr_xCuO_4$ and $Bi_2Sr_2CaCu_2O_{8+\delta}$ display an universal behavior of $T^\ast/T_c$ as a function of hole(positive charge) doping $\delta/\delta_o$ with $\delta_o$, the optimal doping rate, as is shown in Fig.1. Earlier Nakano et al found another type of universality by pointing out that the observed spin gap temperature $T^\ast$ scaled by the maximum superconducting transition temperature $T_c^{\max}$ at optimal doping, $T^\ast/T_c^{\max}$ as a function of doping scaled by the optimal doping, $\delta/\delta_o$ falls on the same curve for the two different high $T_c$ cuprates above. The two observations manifest the presence of a relationship between the spin gap (relevant to the spin degree of freedom) and the superconductivity (related to the charge degree of freedom). Thus, the spinon pairing/spin singlet pairing for pseudogap phase and the charge pairing/holon pairing for superconductivity are not independent owing to the manifest presence of coupling between the charge and spin degrees of freedom.

Various U(1) slave-boson approaches to the t-J Hamiltonian were able to predict such a linear decrease in the pseudogap temperature as a function of $\delta$. In our earlier U(1) slave-boson study, we presented a phase diagram based on the allowance of holon pairing channel, thus showing the feature of the holon-pair Bose condensation temperature rather than the single-holon Bose condensation temperature. On the other hand, all of these theories failed to predict the experimentally observed Bose condensation temperature $T_c$ of the arch shape as a function of $\delta$. Instead a linear increase of $T_c$ with $\delta$ was predicted. Further the pseudogap phase was shown to disappear when the gauge fluctuations are introduced into the U(1) slave-boson mean field theory. Most recently Wen and Lee proposed an SU(2) theory to readily estimate the low energy phase fluctuations of order parameters and made a brief discussion on the possibility of holon(boson) pair condensation. In view of failure in the correct prediction of the Bose condensation temperature $T_c$ in the phase diagram with earlier theories, in the present study we examine the variation of the holon-pair condensation temperature with the hole doping rate, by treating the phase fluctuations of the order parameters in the SU(2) slave boson theory. We realize from the aforementioned observation of the universality in $T^\ast/T_c$ vs. $\delta/\delta_o$ for high $T_c$ cuprates that coupling between the spin(spinon) and charge(holon) degrees of freedom is essential for superconductivity. Our theoretical derivation from the use of the slave-boson theory for t-J Hamiltonian manifests this feature as is shown in the fourth term of the effective Hamiltonian in Eq.(4). In addition, comparison between the two approaches will be made to reveal the importance of the low energy phase fluctuations of the order parameters. The present work differs from our previous U(1) slave-boson study(of the phase diagram involving the holon-pair Bose condensation) and other earlier studies involving the single holon condensation in that coupling between the holon and spinon degrees of freedom in the slave-boson representation of the Heisenberg term of the t-J Hamiltonian is no longer neglected. We find from the treatment of the coupling that the predicted phase diagram displays the arch-shaped Bose condensation curve(temperature $T_c$) as a function of hole doping.
rate in both treatments of the U(1) and SU(2) slave-boson approaches.

We write the t-J Hamiltonian,

$$H = -t \sum_{<i,j>} \left[ \langle c_i^\dagger c_j \rangle + \frac{1}{4} n_i n_j \right].$$

(1)

Here $S_i$ is the electron spin operator at site $i$, $S_i = \frac{1}{2} c_i^\dagger \sigma_{\alpha\beta} c_{i\alpha}$ with $\sigma_{\alpha\beta}$ the Pauli spin matrix element and $n_i$ the electron number operator at site $i$, $n_i = c_i^\dagger c_i$. We note that $S_i \cdot S_j - \frac{1}{2} n_i n_j = -\frac{1}{2} \langle c_i^\dagger c_j \rangle$ in the U(1) slave-boson representation. It should be emphasized that the derivation of $P(S_i \cdot S_j - \frac{1}{2} n_i n_j) = -\frac{1}{2} \langle b_i^\dagger b_j \rangle$ in the U(1) slave-boson representation is correct based on the U(1) slave-boson constraint and that most importantly physics demands the presence of this four boson operator $b_i^\dagger b_i^\dagger b_j^\dagger b_j$ to represent the charge degree of freedom, in addition to the four fermion operator which represents the spin degree of freedom. Each one of $n_i n_j$ and $S_i \cdot S_j$ in the Heisenberg term self-evidently reveals such physics (e.g., note that $n_i$ here represents the electron(or physically the negative charge) number operator). In earlier studies of the slave-boson theory, it is often assumed that $b_i^\dagger b_i^\dagger b_i^\dagger b_i = 1$. Strictly speaking, this is precise only at half-filling (or no hole doping). This is because charge fluctuations cannot occur owing to the prohibition of actual electron hopping from site to site.

By admitting the coupling between the charge and spin degrees of freedom in the SU(2) slave-boson representation, the t-J Hamiltonian above can be written,

$$H = -\frac{t}{2} \sum_{<i,j>} \left[ \langle f_i^\dagger f_j \rangle \langle b_i^\dagger b_j \rangle - \langle b_i^\dagger b_j \rangle \langle f_i^\dagger f_j \rangle \right]$$

Here $f_i$ is the spinon annihilation (creation) operator and $h_i \equiv \left( \begin{array}{c} b_{i1} \\ b_{i2} \end{array} \right)$ is the doublet of holon annihilation (creation) operators. $\chi_{ij}^{(1),(2),(3)}$ are the real Lagrangian multipliers to enforce the local single occupancy constraint in the SU(2) slave-boson representation.

The Heisenberg interaction term (the second term in Eq. (3)) above can be decomposed into terms involving mean fields and fluctuations respectively,

$$-\frac{J}{2} \sum_{<i,j>} \left[ \langle h_i^\dagger h_j \rangle \langle f_{i1}^\dagger f_{j1} \rangle - \langle f_{i1}^\dagger f_{j1} \rangle \langle h_i^\dagger h_j \rangle \right]$$

$$J \sum_{<i,j>} \left[ \langle h_i^\dagger h_j \rangle \langle f_{i1}^\dagger f_{j1} \rangle \langle f_{i2}^\dagger f_{j2} \rangle - \langle f_{i1}^\dagger f_{j1} \rangle \langle f_{i2}^\dagger f_{j2} \rangle \langle h_i^\dagger h_j \rangle \right]$$

(3)
where \( \Delta_{ij} = \langle (f_i f_j - f_{2i} f_{2j}) \rangle = \Delta_{ij}^f - \frac{1}{(1-\delta)} \chi_{ij, 12} \), with \( \chi_{ij, 12} = \langle b_{2i} b_{j} + b_{j}^+ b_{2i} \rangle \) with \( \delta \), hole doping rate. In Eq.\((H)\) above we introduced \( \langle (f_{2i} f_{j} - f_{i} f_{2j}) \rangle \approx \langle (f_{2i} f_{j} - f_{i} f_{2j}) \rangle = |\Delta_{ij}^f|^2 \) and \( \langle (1-h_i^1 h_j^1)(1-h_i^2 h_j^2) \rangle \approx \langle (1-h_i^1 h_j^1) \rangle \langle (1-h_i^2 h_j^2) \rangle = (1-\delta)^2 \) and neglected the last term in Eq.\((H)\) above. The four boson term in the fourth term of Eq.\((4)\) allows holon pairing and a scalar boson field, \( \Delta_{ij; \alpha \beta} \) is introduced for the holon pairing between the nearest neighbor \( b_{\alpha} \)– and \( b_{\beta} \)–single bosons with the boson index, \( \alpha, \beta = 1 \) or \( 2 \). Using the saddle point approximation, we obtain from Eq.\((H)\) the mean field Hamiltonian,

\[
H^{MF} = \frac{J(1-\delta)^2}{2} \sum_{<i,j>} \left| \Delta_{ij}^f \right|^2 \left( \frac{1}{2} \chi_{ij}^1 + \frac{1}{4} \chi_{ij}^2 \right) \\
+ \frac{1}{2} \sum_{<i,j>} \left| \Delta_{ij}^f \right|^2 \left( \sum_{\alpha, \beta} \left| \Delta_{ij; \alpha \beta} \right|^2 + \delta^2 \right) \\
- \frac{J(1-\delta)^2}{4} \sum_{<i,j>} \left[ \chi_{ij} \left( \delta_{ij} (f_i f_{2i} - f_{2i} f_i) + c.c. \right) \right] \\
- \frac{J(1-\delta)^2}{4} \sum_{<i,j>} \left[ \chi_{ij} \left( f_{ij}^f f_{ij} f_{ij} f_{ij} + c.c. \right) \right] \\
- \frac{t}{2} \sum_{<i,j>} \left[ \chi_{ij} (b_{i}^+ b_{j} - b_{i} b_{j}^+) - \Delta_{ij}^f (b_{i}^+ b_{j} + b_{j}^+ b_{i}) \right] - c.c. \\
- \sum_{<i,j>, \alpha, \beta} \frac{J}{2} \left[ \left| \Delta_{ij; \alpha \beta} \right|^2 (b_{\alpha i} b_{\alpha j} + b_{\beta i} b_{\beta j}) + c.c. \right] \\
- \sum_{i} \left[ \mu_i (h_i^1 h_i^1 - \delta) + i\lambda_i^1 (f_i f_{2i} + b_i^+ b_{2i}) \right] \\
+ i\lambda_i^2 (f_{2i} f_{2i} + b_{2i} b_{2i}) + i\lambda_i^3 (f_{i} f_{2i} - f_{2i} f_i + b_{i}^+ b_{2i} + b_{2i}^+ b_{i}) \right] \\
- \frac{t}{2} \sum_{<i,j>} \left[ \chi_{ij} \left( \delta_{ij} (f_{ij} f_{ij} - f_{2ij} f_{2ij}) + c.c. \right) \right] \\
+ \frac{t}{2} \sum_{<i,j>} \left[ \chi_{ij} \left( f_{ij} f_{ij} f_{ij} f_{ij} + c.c. \right) \right] \\
+ \frac{t}{2} \sum_{<i,j>} \left[ \chi_{ij} \left( b_{i} b_{j} - b_{i}^+ b_{j}^+ \right) \right] \chi_{ij} \left( b_{i}^+ b_{j} + b_{j}^+ b_{i} \right)
\]

\[(5)\]

where \( \chi_{ij} = \langle f_{ij}^f f_{ij}^f \rangle \), \( \chi_{ij, 12} = \langle b_{2i} b_{j} + b_{j}^+ b_{2i} \rangle \), \( \Delta_{ij}^f \) \( \langle f_{ij} f_{ij} - f_{2ij} f_{2ij} \rangle \), \( \Delta_{ij}^b \) \( \langle b_{ij} b_{ij} - b_{ij}^+ b_{ij}^+ \rangle \). The Hubbard Stratonovich field \( \rho_{ij}^{(k)} = \langle f_{ij}^f \rangle \) for direct channel is taken to be 0 \( \notin \) and \( \rho_{ij}^{(k)} = \frac{1}{2} \). Owing to the energy cost the exchange interaction terms(the last two positive energy terms in Eq.\((H)\)) is usually ignored \( \notin \) \( \notin \).

(4) We now introduce the uniform hopping order parameter, \( \chi_{ij} = \chi \), the d-wave spinon pairing order parameter, \( \Delta_{ij}^d = \pm \Delta \) with the sign (+) for the nearest neighbor link parallel to \( \hat{x} \) (\( \hat{y} \)) and the s-wave holon pairing order parameter, \( \Delta_{ij; \alpha \beta} = \Delta_{ij; \alpha \beta} \) with the boson indices \( \alpha \) and \( \beta \). For the case of \( \Delta_{ij; \alpha \beta} = 0 \), \( \chi(k) = 0 \) and \( \Delta^d \leq \chi \), the \( b_{1} \)-bosons are populated at and near \( k = (0, 0) \) in the momentum space and the \( b_{2} \)-bosons, at and near \( k = (\pi, \pi) \) \( \notin \). Pairing of two different(\( \alpha \neq \beta \)) bosons(holons) gives rise to the non-zero center of mass momentum. On the other hand, the center of mass momentum is zero only for pairing between identical(\( \alpha = \beta \)) bosons. Thus writing \( \Delta_{ij; \alpha \beta} = \Delta_{ij; \alpha \beta} \) \( \notin \) for pairing between the identical holons and allowing the uniform chemical potential, \( \mu = \mu \), the mean field Hamiltonian from Eq.\((H)\) is derived to be,

\[
H^{MF} = NJ(1-\delta)^2 \left( \frac{1}{2} \lambda^2 + \Delta^2 + \frac{1}{4} \right) + NJ \Delta^2 / 4(2 \Delta^2 + \delta^2) \\
+ \sum_{k} E_k^f (\alpha_{k1}^1 \alpha_{k1}^1 - \alpha_{k2} \alpha_{k2}^1) \\
+ \sum_{k, s=1, 2} E_{ks}^b \beta_{ks} \beta_{ks} + \frac{1}{2} (E_{ks}^b + \mu) \right] + \mu N \delta. \]

\[(6)\]

Here \( E_k^f \) and \( E_{ks}^b \) are the quasiparticle energies of spinon and holon respectively, \( \alpha_{ks} (\alpha_{ks})^1 \) and \( \beta_{ks} (\beta_{ks})^1 \) are the annihilation(creation) operators of the spinon quasiparticles and the holon quasiparticles respectively.

From the diagonalized Hamiltonian Eq.\((H)\), we readily obtain the total free energy,

\[
F = NJ(1-\delta)^2 \left( \frac{1}{4} + \Delta^2 + \frac{1}{2} \chi^2 \right) \\
- 2k_B T \sum_{k} ln(cosh(\beta E_k^f / 2)) \\
+ NJ \Delta^2 (\Delta^2 + \delta^2) + k_B T \sum_{k, s} ln[1 - e^{-\beta E_{ks}^b}] \\
+ \sum_{k, s=1, 2} \frac{E_{ks}^b + \mu}{2} + \mu N \delta. \]

\[(7)\]

The chemical potential is determined from the number constraint of doped holes,

\[
- \frac{\partial F}{\partial \mu} = \sum_{k} \left[ \frac{1}{e^{\beta E_k^f} - 1} - \frac{e_k^f - \mu}{E_k^f} + \frac{1}{2} \left( \frac{e_k^f - \mu}{E_k^f} - 1 \right) \right] \\
+ \frac{1}{e^{\beta E_{ks}^b} - 1} - \frac{e_{ks}^b - \mu}{E_{ks}^b} + \frac{1}{2} \left( \frac{e_{ks}^b - \mu}{E_{ks}^b} - 1 \right) \right] - N \delta = 0. \]

\[(8)\]

and the Lagrangian multipliers are determined by the following three constraints imposed by the SU(2) slave-boson theory,

\[
\frac{\partial F}{\partial \lambda(k)} = - \sum_{k} \Lambda \left( \frac{\beta E_k^f}{2} - \frac{\beta E_k^f}{2} \right) \frac{\partial \lambda(k)}{\partial \lambda(k)}
\]

\[3\]
It can be readily proven from Eq. (10) above that \( \lambda(k) = 0 \) satisfies the three constraints above.

By minimizing the free energy, the order parameters \( \chi, \Delta_f \) and \( \Delta_b \) are numerically determined as a function of temperature and doping rate. In Fig. 2 the mean field results of the U(1) slave-boson theory (dotted lines) are displayed for \( J = 0.2 \text{ t} \), \( J = 0.3 \text{ t} \) and \( J = 0.4 \text{ t} \) for comparison with the predicted phase diagrams (solid lines). The predicted pseudogap (spin gap) temperature, \( T_{SU(2)} \) is consistently higher than \( T_{U(1)} \) (the U(1) value). \( T_{SU(2)} \) at optimal doping rate is shifted to a larger value, showing closer agreement with observation [1][2][3] than the U(1) mean field treatment. Such discrepancies are attributed to the phase fluctuations of order parameters, which were not treated in the U(1) mean field theory. We note from the four boson operator \(-\frac{1}{2} \Delta^b_{ij} b^i \alpha b^j \beta b^\alpha b^\beta \) in the fourth term of Eq. (4) that the strength of holon pairing depends on the spinon pairing amplitude (order parameter) \( \Delta^b_{ij} \). According to the predicted holon pair condensation temperature (superconducting transition temperature) \( T_{SU(2)} \) depends on the spin gap (pseudogap) temperature \( T^* \); \( T_{SU(2)} \) decreases with \( T^* \) in the overdoped region. Indeed it is shown in Eq. (2) that the predicted holon pair condensation temperature \( T_{c} = T_{SU(2)} \) is not independent of the spin gap (pseudogap) formation at \( T^* \), by exhibiting the diminishing trend of superconducting temperature \( T_c \) as the spin gap temperature \( T^* \) decreases in the overdoped region. This is consistent with an experimental observation of the universal behavior of \( T^*/T_c \) as a function of hole doping rate \( \delta / \delta_0 \) for different high \( T_c \) cuprates, as shown in Fig. 1.

In summary, based on the SU(2) slave-boson symmetry conserving t-J Hamiltonian which shows coupling between the charge and spin degrees of freedom, we derived a phase diagram of high \( T_c \) cuprates which displays the bose condensation temperature of an arch shape as a function of hole doping rate. Unlike other previous studies which predicted a linear increase with the hole doping rate, this result is consistent with observation. We showed that the low energy fluctuations cause a shift of the optimal doping rate to a larger value and a suppression of the holon pair Bose condensation temperature, thus allowing a closer agreement with observation compared to the U(1) case.

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[8] We show the presence of four boson operator of the form \((1-h^\dagger_1 h^\dagger_2)(1-h^\dagger_3 h^\dagger_4)\) is essential in the SU(2) representation, and the four boson operator leads to \(\chi^*\). It is of note that the electron (negative charge) number operator is always wrong. Consider a matrix element for the state |ahr > with holons (bosons) at both sites i and j. We readily note that its matrix element of \((S_i \cdot S_j - \frac{1}{2} n_i n_j)\) is 0, i.e., <ahr | \(\frac{1}{2}(c^i_\downarrow c^i_\uparrow - c^i_\downarrow c^j_\uparrow)(c^j_\uparrow c^i_\uparrow - c^j_\downarrow c^i_\downarrow)\) |ahr > = 0 in the electron representation. In the SU(2) slave-boson theory, the holon pair state is given by |ahr > = \(\frac{1}{2}(b^i_\dagger + b^j_\dagger f^i_\dagger f^j_\dagger f^i_\downarrow f^j_\uparrow |ahr > \). With the presence of the four boson operator the matrix element for the holon pair state in the SU(2) slave-boson representation is correctly, <ahr | \(-\frac{1}{2}(1-h^\dagger_1 h^\dagger_2)(1-h^\dagger_3 h^\dagger_4)(f^i_\dagger f^j_\dagger f^i_\dagger f^j_\downarrow)(f^j_\dagger f^j_\dagger f^j_\dagger f^j_\uparrow)\) |ahr > = 0. On the other hand, the matrix element involving only the four fermion operator is erroneously, <ahr | \(-\frac{1}{2}(f^i_\dagger f^j_\dagger f^i_\dagger f^j_\dagger)(f^j_\dagger f^j_\dagger f^j_\dagger f^j_\uparrow)\) |ahr > = \(-\frac{1}{2}\). Therefore, the four boson operator \((1-h^\dagger_1 h^\dagger_2)(1-h^\dagger_3 h^\dagger_4)\) should be retained. The term \((S_i \cdot S_j - \frac{1}{2} n_i n_j)\) is reduced to \(-b^i_\dagger b^j_\dagger b^j_\dagger b^i_\dagger f^i_\dagger f^j_\dagger f^j_\dagger f^i_\downarrow(f^j_\dagger f^j_\dagger f^j_\dagger f^j_\uparrow)\) in the U(1) representation (Proof: In the U(1) representation we note that the holon part \((1-h^\dagger_1 h^\dagger_2)(1-h^\dagger_3 h^\dagger_4)\) leads to \((1-b^i_\dagger b^j_\dagger)(1-b^j_\dagger b^i_\dagger)\). Realizing \(1-b^i_\dagger b^j_\dagger = b^i_\dagger b^j_\dagger\), we find that \((1-b^i_\dagger b^j_\dagger)(1-b^j_\dagger b^i_\dagger) = b^i_\dagger b^j_\dagger b^j_\dagger b^i_\dagger\). Note that \(b^i_\dagger b^j_\dagger\) acts as an electron (negative charge -e) number operator but not as the holon number operator of positive charge +e. It is obvious that the value of \(b^i_\dagger b^j_\dagger\) is 1 for an electron occupied at site i and 0 for the occupation of the holon (hole) at site i. It is of note that the electron (negative charge) number operator is always \(b^i_\dagger b^j_\dagger = 1 - b^i_\dagger b^j_\dagger \leq 1\).
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FIG. 1. $T^*/T_c$ vs $\delta/\delta_0$ for $La_{2-x}Sr_xCuO_4$ and $Bi_2Sr_2CaCu_2O_{8+\delta}$. The solid line represents a fitted curve by $T^*/T_c = (\delta/\delta_0)^a + b$ with $a = -1.86$ and $b = 0.69$. Data points are taken from the paper of Nakano et al[2].

FIG. 2. Computed phase diagrams with $J = 0.2t$, $J = 0.3t$ and $J = 0.4t$. $T_{SU(2)}^f(T_{U(1)}^f)$ denotes the pseudogap temperature and $T_{SU(2)}^p(T_{U(1)}^p)$, the holon pair bose condensation temperature predicted from the SU(2)(solid lines) and (U(1))(dotted lines) slave-boson theories respectively. The scale of temperature in the figure is based on $t = 0.44eV$[9].