Study of d-wave Hole Pairing and Supersymmetry Condition Based on the U(1) Slave Boson Theory of t-J Hamiltonian

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Abstract

Based on the local U(1) gauge slave-boson approach to the t-J Hamiltonian, we examine a possibility of hole pairing at finite temperature and hole doping rate. It is found that as a result of symmetry breaking d-wave holon pairing with finite gap can occur. In addition a holon-spinon supersymmetry condition at $T = 0K$ is obtained based on spinon and holon excitations at a critical doping region between antiferromagnetic and superconducting phases.

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Slave-boson approach to the t-J Hamiltonian is often employed for the study of strongly correlated electron systems, including high T_C cuprates. In the mean field level [1], the superconducting order parameter $< c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger >$ is taken to be $< b_i b_j >< f_{i\uparrow}^\dagger f_{j\downarrow}^\dagger >$. This suggests that the superconducting state occurs only when both spinon and holon pairs are condensed simultanesouly. Recently, SU(2) slave-boson theory was employed in the t-J Hamiltonian to probe the possibility of single holon and holon pair condensations [2]. In the present study we closely follow earlier studies of the U(1) slave-boson approach advanced by Ubbens and Lee [3] and explore a possibility of d-wave hole pairing for hole-doped cuprates. We also explore a spinon-holon supersymmetry condition in the context of quasi particle excitation spectrum.

The t-J Hamiltonian in the local U(1) gauge slave-boson form [1], [3] is written

$$\begin{aligned} H = & -t \sum_{<i,j>} (f_{i\sigma}^\dagger f_{j\sigma} b_j^\dagger b_i + c.c.) \\ & + J \sum_{<i,j>} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j) - \mu_0 \sum_{i,\sigma} f_{i\sigma}^\dagger f_{i\sigma} \\ & + i \sum_i \lambda_i (f_{i\sigma}^\dagger f_{i\sigma} + b_i^\dagger b_i - 1), \end{aligned} \tag{1}$$

where $f_{i\sigma}(f_{i\sigma}^\dagger)$ is the spinon annihilation(creation) operator; $b_i(b_i^\dagger)$, the holon annihilation(creation) operator; and n_i, the electron(spinon) number operator at site i. λ_i is the Lagrangian multiplier to enforce local single occupancy constraint. $\mathbf{S}_i$ is the electron spin operator at site i, $\mathbf{S}_i = \frac{1}{2} f_{i\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} f_{j\beta}$ with $\boldsymbol{\sigma}_{\alpha\beta}$, the Pauli spin matrix element.

The Heisenberg term can be decoupled into Hatree-Fock-Bogoliubov channels in association with the direct, exchange and pairing interactions, by introducing corresponding Hubbard-Stratonovich fields, $\boldsymbol{\rho}_i^f$, χ_{ji}^f and Δ_{ji}^f. The resulting effective Hamiltonian with the inclusion of the hopping term is [3],

$$\begin{aligned} H = & \frac{3J}{8} \sum_{<i,j>} \Big[|\chi_{ji}|^2 + |\Delta_{ji}^f|^2 - \chi_{ji}^* \Big(f_{j\sigma}^\dagger f_{i\sigma} + \frac{8t}{3J} b_j^\dagger b_i \Big) - c.c. + n_i \\ & - \Delta_{ji}^{f*} (f_{j\uparrow} f_{i\downarrow} - f_{j\downarrow} f_{i\uparrow}) - c.c. \Big] + \frac{J}{2} \sum_{<i,j>} \Big(|\boldsymbol{\rho}_i^f|^2 - \sum_{k=1}^{3} (\rho_i^f)^k (f_j^\dagger \sigma^k f_j) \Big) \\ & - \mu_0 \sum_i f_{i\sigma}^\dagger f_{i\sigma} - i \sum_i \lambda_i (f_{i\sigma}^\dagger f_{i\sigma} + b_i^\dagger b_i - 1) \\ & + \frac{8t^2}{3J} \sum_{<i,j>} b_j^\dagger b_i b_i^\dagger b_j - \frac{J}{4} \sum_{<i,j>} n_i n_j. \end{aligned} \tag{2}$$

In the above expression the last two terms were neglected in the previous work (Eq.(4) in [3]). They are needed in order to properly describe the physics of hole pairing for the hole-doped cuprates of present interest. It is of note that the added term,$\sum_{<i,j>} b_j^\dagger b_i b_i^\dagger b_j$ is associated only with the exchange interaction channel.

The introduction of $n_i = 1 - b_i^\dagger b_i$(with neglect of double occupancy) and the Hartree-Fock-Bogoliubov channels into the last term in Eq.(2) leads to

$$e^{\frac{J}{4}\sum_{<i,j>} n_i n_j} = e^{\frac{J}{4}\sum_{<i,j>} b_i^\dagger b_j^\dagger b_i b_j - J\sum_i b_i^\dagger b_i + \frac{NJ}{2}}$$
$$\propto \int \prod_i d\rho_i^b \prod_{<i,j>} d\chi_{ji}^{b*} d\chi_{ji}^b d\Delta_{ji}^{b*} d\Delta_{ji}^b e^{-\sum_{<i,j>} B_{ji}}, \tag{3}$$

where

$$B_{ji} = \frac{J}{12}\Big[(\rho_i^b)^2 - 2\rho_i^b(b_j^\dagger b_j) + |\chi_{ji}^b|^2 - \chi_{ji}^{b*}(b_j^\dagger b_i) - c.c + |\Delta_{ji}^b|^2 - \Delta_{ji}^{b*}(b_j b_i) - c.c\Big] + \frac{7J}{6}\sum_i b_i^\dagger b_i - \frac{NJ}{2}.$$

Here $b_i^\dagger b_j^\dagger b_i b_j$ is decomposed into Hartree, Fock and Bogoliubov channels by equally weighting them. ρ^b, χ^b and Δ^b are the Hubbard-Stratonovich fields corresponding to the direct, exchange and pairing channels respectively. N is the total number of sites or the total number of electrons at half-filling.

We obtain the mean field Hamiltonian from Eqs.(2) and (3) by using the saddle point approximation,

$$H^{MF} = \sum_{<i,j>}\Big[\frac{3J}{8}\Big(|\Delta_{ji}^f|^2 + |\chi_{ji}^f|^2\Big) + \frac{J}{12}\Big(|\Delta_{ji}^b|^2 + |\chi_{ji}^b|^2 + (\rho_i^b)^2\Big) + t\Big(\chi_{ji}^f\chi_{ji}^{b*} + \chi_{ji}^{f*}\chi_{ji}^b\Big)\Big]$$
$$-\frac{3J}{8}\sum_{<i,j>}\Big[\Delta_{ji}^*(f_{j\uparrow}f_{i\downarrow} - f_{j\downarrow}f_{i\uparrow}) + c.c.\Big] - \frac{3J}{8}\sum_{<i,j>}\Big[\Big(\chi_{ji}^f + \frac{8t}{3J}\chi_{ji}^b\Big)^*(f_{j\sigma}^\dagger f_{i\sigma}) + c.c.\Big]$$
$$+\frac{J}{2}\sum_{<i,j>}\Big(|\boldsymbol{\rho}_i^f|^2 - \sum_{k=1}^{3}(\rho_i^f)^k(f_j^\dagger\sigma^k f_j)\Big) - \sum_{i,\sigma}\mu_i^f(f_{i\sigma}^\dagger f_{i\sigma})$$
$$-t\sum_{<i,j>}\Big[\Big(\chi_{ji}^f + \frac{J}{12t}\chi_{ji}^b\Big)^*(b_j^\dagger b_i) + c.c.\Big] - \frac{J}{12}\sum_{<i,j>}\Big[\Delta_{ji}^{b*}(b_i b_j) + c.c.\Big] - \sum_i \mu_i^b(b_i^\dagger b_i)$$
$$+\frac{8t^2}{3J}\sum_{<i,j>}(b_j^\dagger b_i - \chi_{ji}^b)(b_i^\dagger b_j - \chi_{ji}^{b*}). \tag{4}$$

Here the saddle-point(mean) values of interest are given by $\chi_{ji}^f =< f_{j\sigma}^\dagger f_{i\sigma} >$, $\chi_{ji}^b =< b_j^\dagger b_i >$, $\Delta_{ji}^f =< f_{j\uparrow}f_{i\downarrow} - f_{j\downarrow}f_{i\uparrow} >$, $\Delta_{ji}^b =< b_j b_i >$, $\rho_i^b =< b_i^\dagger b_i >= \delta_i$ and $\boldsymbol{\rho}_i^f =< \mathbf{S}_i >$. $\boldsymbol{\rho}_i^f$ will be taken to be 0 as in Ref. [3]. The effective chemical potentials are defined by $\mu_i^f = \mu_0 + i\lambda_i - 3J/4$ for spinons and $\mu_i^b = i\lambda_i + \frac{J}{3}\rho_i^b - 7J/6$ for holons.

Following Ubbens and Lee [3] we now set for the order parameters in Eq.(4),

$$\chi^f_{ji} = \chi^f e^{\pm i\theta^f} \text{ and } \chi^b_{ji} = \chi^f e^{\pm i\theta^b}, \tag{5}$$

where the sign $+(-)$ is along(against) the arrow(see Fig. 6),

$$\Delta^f_{ji} = \Delta^f e^{\pm i\tau^f} \text{ and } \Delta^b_{ji} = \Delta^b e^{\pm i\tau^b}, \tag{6}$$

where the sign $+(-)$ is for the **ij** link parallel to $\hat{x}$ ($\hat{y}$). We allow uniform(site-independent) chemical potentials, $\mu^f_i = \mu^f$ and $\mu^b_i = \mu^b$. Applying Bogoliubov-Valatin transformation after the momentum space transformation of the mean field Hamiltonian H^{MF} above, we obtain the following diagonalized Hamiltonian,

$$\begin{aligned} H^{MF} = & \frac{3NJ}{4}\Big((\Delta^f)^2 + (\chi^f)^2\Big) + \sum_{k,s=\pm1}^{\prime} E^f_{ks}(\alpha^\dagger_{ks}\alpha_{ks} - \beta_{ks}\beta^\dagger_{ks}) - N\mu^f \\ & + \frac{NJ}{6}\Big((\Delta^b)^2 + (\chi^b)^2 + (\rho^b)^2\Big) + \sum_{k,s=\pm1}^{\prime} \{E^b_{ks}(h^\dagger_{ks}h_{ks} + \frac{1}{2}) - \frac{\epsilon^b_{ks}}{2}\} + \frac{N\mu^b}{2} \\ & + 4Nt\chi^f\chi^b\cos(\theta^f - \theta^b). \end{aligned} \tag{7}$$

Here the quasi particle energies are given by

$$E^f_{ks} = \sqrt{(\epsilon^f_{ks} - \mu^f)^2 + \Big(\frac{3J}{4}\xi_k(\tau^f)\Delta^f\Big)^2}, \tag{8}$$

for the spinon and

$$E^b_{ks} = \sqrt{(\epsilon^b_{ks} - \mu^b)^2 - \Big(\frac{J}{6}\xi_k(\tau^b)\Delta^b\Big)^2}, \tag{9}$$

for the holon, where

$$E^{b'}_{ks} = \frac{1}{2}\Big(E^b_{ks} - (\epsilon^b_{ks} - \mu^b)\Big), \tag{10}$$

$$\epsilon^f_{ks} = \frac{3}{4}sJ\sqrt{\gamma^2_k\Big(\chi^f\cos\theta^f + \frac{8t}{3J}\chi^b\cos\theta^b\Big)^2 + \varphi^2_k\Big(\chi^f\sin\theta^f + \frac{8t}{3J}\chi^b\sin\theta^b\Big)^2}, \tag{11}$$

$$\epsilon^b_{ks} = 2st\sqrt{\gamma^2_k\Big(\chi^f\cos\theta^f + \frac{J}{12t}\chi^b\cos\theta^b\Big)^2 + \varphi^2_k\Big(\chi^f\sin\theta^f + \frac{J}{12t}\chi^b\sin\theta^b\Big)^2}, \tag{12}$$

$$\xi_k(\tau) = \sqrt{\gamma^2_k\cos^2\tau + \varphi^2_k\sin^2\tau}, \text{with } \tau = \tau^f \text{ or } \tau^b \tag{13}$$

$$\gamma_k = (\cos k_x + \cos k_y), \tag{14a}$$

$$\varphi_k = (\cos k_x - \cos k_y). \tag{14b}$$

$\alpha_{ks}(\alpha_{ks}^\dagger)$ and $\beta_{ks}(\beta_{ks}^\dagger)$ are the annihilation(creation) operators of spinon quasiparticle and $h_{ks}(h_{ks}^\dagger)$, the annihilation(creation) operators of holon quasiparticle. $\sum_k'$ denotes a sum over half of the Brillouin zone. In deriving the expression (7), fluctuations of holon hopping order, $(b_j^\dagger b_i - < b_j^\dagger b_i >)$ which appears in the last term of Eq.(4) are neglected.

Using the diagonalized Hamiltonian(7), we readily obtain the free energy,

$$
\begin{aligned}
F = & \frac{3NJ}{4}\Big((\Delta^f)^2 + (\chi^f)^2\Big) - 2k_BT \sum_{k,s=\pm1}^{\prime} ln[\cosh(\beta E_{ks}^f/2)] - N\mu^f - 2Nk_BTln2 \\
& + \frac{NJ}{6}\Big((\Delta^b)^2 + (\chi^b)^2 + \delta^2\Big) + k_BT \sum_{k,s=\pm1}^{\prime} ln[1 - e^{-\beta E_{ks}^b}] + \sum_{k,s=\pm1}^{\prime} \frac{E_{ks}^b - \epsilon_{ks}^b}{2} + \frac{N\mu^b}{2} \\
& + 4Nt\chi^f\chi^b\cos(\theta^f - \theta^b).
\end{aligned} \tag{15}
$$

It is of note that the neglect of δ, Δ^b and χ^b and rescaling of all energies by $\frac{3J}{4}$ leads to the same result(Eq.(11) in [3]) obtained by Ubbens and Lee. By properly choosing the phases of the order parameters in Eqs.(5) and (6) and minimizing the free energy, the amplitudes of the order parameters(χ's and Δ's) can be determined as a function of temperature and doping rate [1], [3]. The chemical potential at finite temperature is determined from the use of Eq.(15), that is, $\frac{\partial F}{\partial \mu^b} = -N\delta$ for holon and $\frac{\partial F}{\partial \mu^f} = -N(1-\delta)$ for spinon. Here we pay attention only to the equations concerned with holon pairing and holon chemical potential, μ^b

$$
\frac{\partial F}{\partial \Delta^b} = \frac{J}{3}\Delta^b\Big[N - \sum_{k,s=\pm1}^{\prime}\Big(\frac{1}{e^{\beta E_{ks}^b} - 1} + \frac{1}{2}\Big)\frac{J\xi_k(\tau^b)^2}{12E_{ks}^b}\Big] = 0, \tag{16}
$$

$$
-\frac{\partial F}{\partial \mu^b} = \sum_{k,s=\pm1}^{\prime}\Big[\frac{1}{e^{\beta E_{ks}^b} - 1}\frac{\epsilon_{ks}^b - \mu^b}{E_{ks}^b} + \frac{\epsilon_{ks}^b - \mu^b - E_{ks}^b}{2E_{ks}^b}\Big] = N\delta. \tag{17}
$$

It is gratifying to find that the first expression Eq.(16) $\frac{\partial F}{\partial \Delta^b} = 0$ is readily satisfied for the holon pairing order, $\Delta^b = 0$, indicating the symmetry with respect to the free energy of holon(holon sector) in Eq.(15) and the second one Eq.(17) leads to to the correct statistical relation for free holon, $\sum_{k,s=\pm1}^{\prime} \frac{1}{e^{\beta(\epsilon_{ks}^b - \mu^b)} - 1} = N\delta$. In order to explore a possibility that this symmetry is spontaneously broken, we now examine the condition for

$$
\frac{\partial^2 F}{\partial \Delta^{b2}}\Big|_{\Delta^b=0} = \frac{J}{3}\Big[N - \sum_{k,s=\pm1}^{\prime}\Big(\frac{1}{e^{\beta(\epsilon_{ks}^b - \mu^b)} - 1} + \frac{1}{2}\Big)f_s(k;\tau^b)\Big] < 0 \tag{18}
$$

where $f_s(k;\tau^b) = \frac{J\xi_k(\tau^b)^2}{12(\epsilon_{ks}^b - \mu^b)}$. As temperature increases, the second term in Eq.(18) becomes smaller with increasing value of $\epsilon_{ks}^b - \mu^b$, thus allowing a possibility of $\frac{\partial^2 F}{\partial \Delta^{b2}} \geq 0$. On the other hand, as temperature decreases, $\epsilon^b_{ks} - \mu^b$ decreases, which results in a possibility of $\frac{\partial^2 F}{\partial \Delta^{b2}} < 0$. We note that $0 \le \xi_k(\tau^b) \le 2$ from Eqs.(13) through (14b). For the d-wave($\tau^b = \pi/2$), $\xi_k(\tau^b)$ is maximized at van-Hove singularities, $\mathbf{k} = (0, \pm\pi)$ and $(\pm\pi, 0)$ (but vanishes at $\mathbf{k} = (0,0)$, $(\pm\pi/2, \pm\pi/2)$ and $(\pm\pi, \pm\pi)$), thus allowing a possibility of instability against d-wave holon pairing with a finite gap, $\Delta^b \neq 0$ owing to $\frac{\partial^2 F}{\partial \Delta^{b2}} < 0$. Thus for both the spinon and holon hopping order parameters χ_{ji} of the 2π-flux phase($\theta^f = \theta^b = \pi/2$) and for the d-wave($\tau^b = \pi/2$) holon pairing order parameter Δ^b_{ji}, $f_s(k;\tau^b)$ is maximized. Consequently the gapless state ($\Delta^b = 0$) can become unstable against the d-wave holon pairing with a finite gap, $\Delta^b \neq 0$. Thus as a result of symmetry breaking, the gap opening of d-wave holon-pairing is possible to induce bose condensation.

To numerically confirm claims made above, we calculated $\frac{\partial^2 F}{\partial \Delta^{b2}}$ for d-wave pairing for both spinon pair and holon pair by setting $\chi^f = \chi^b$ and $\tau^b = \pi/2$. It is of note that arbitrary variation of χ^f and χ^b does not affect qualitative discussions to be made below. Here the hopping order parameter is assumed to remain independent of doping. Kotliar and Liu [1] finds a nearly constant value of $\chi^f \approx \frac{1}{3}$. As the doping rate decreases, the critical temperature at which instability against d-wave holon pairing begins to develop is predicted to decrease. Such a lowering trend of the critical temperature is consistent with observations in the underdoped region [4] [5]. In Fig.6 the area above each curve for each chosen value of the hopping order parameter represents the region for $\frac{\partial^2 F}{\partial \Delta^{b2}} > 0$ and the area below the curves, $\frac{\partial^2 F}{\partial \Delta^{b2}} < 0$.

We now pay attention to holon and spinon quasi-particle excitations based on the mean field Hamiltonian in Eq.(7),

$$H = \sum_{k,s=\pm 1}{}' E_{ks}(\alpha^\dagger_{ks}\alpha_{ks} + \beta^\dagger_{ks}\beta_{ks} + h^\dagger_{ks}h_{ks}). \tag{19}$$

for $E_{ks} = E^f_{ks} = E^b_{ks}$. The condition of $E^f_{ks} = E^b_{ks}$ is satisfied from Eqs.(8) and (9) when

$$\Delta^f = \Delta^b = 0, \tag{20}$$

$$\chi^f = \chi^b = 0, \tag{21}$$

$$\mu^f = \mu^b. \tag{22}$$

It is, also, worthy of note that with the neglect of constant terms that appear in Eq.(7) the SUSY(supersymmetry) Hamiltonian in Eq.(19) is naturally obtained from the above supersymmetry conditions of Eqs.(20) through (22). Accordingly we are now able to define the supercharge operators,

$$Q = \sum_{k,s=\pm 1}^{\prime} \sqrt{\frac{E_{ks}}{2}} \Big(\alpha^{\dagger}_{ks} h_{ks} + h^{\dagger}_{ks} \alpha_{ks} \Big), \tag{23}$$

which, in turn, satisfies the simple SUSY algebra

$$\{Q, Q\} = \sum_{k,s=\pm 1}^{\prime} E_{ks} (\alpha^{\dagger}_{ks} \alpha_{ks} + h^{\dagger}_{ks} h_{ks}). \tag{24}$$

Particularly at $T = 0$ the SUSY condition of expressions (20) through (22) may be better met in the doping region of $\delta_{A.F.} < \delta < \delta_{S.C.}$ with $\delta_{A.F.}$, the upper limit of doping for the antiferromagnetic phase and $\delta_{S.C.}$, the lower limit of doping for the superconducting phase (see Fig.6) [4] [6]. This is the region where quantum fluctuation occur to allow $\Delta^f = \Delta^b = 0$ and holon(charge) and spinon(spin) separation is likely to occur.

In summary, by considering the complete t-J Hamiltonian with the inclusion of the energy lowering term, $-\frac{J}{4} n_i n_j$, it is shown that at finite temperature bose condensation owing to d-wave holon pairing with a finite gap can occur. A holon-spinon supersymmetry condition is obtained based on the quasiparticle excitations for both holons and spinons.

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FIGURE CAPTIONS

Fig. 1. Flux phases of hopping and pairing order parameters. (a) $+\theta(-\theta)$ along(against) the arrow on the chain. (b) $+\tau(-\tau)$ in the chain of $\hat{x}(\hat{y})$ direction.

Fig. 2. Critical temperature of d-wave holon pairing as a function of doping rate for various values of $\chi^f = \chi^b$ and $\theta^f = \theta^b = \pi/2$. $\frac{\partial^2 F}{\partial \Delta^{b2}} > 0$ above each curve and $\frac{\partial^2 F}{\partial \Delta^{b2}} < 0$ below the curve.

Fig. 3. Schematic phase diagram of $La_{2-\delta}Sr_\delta CuO_4$(Ref.[4][6]).

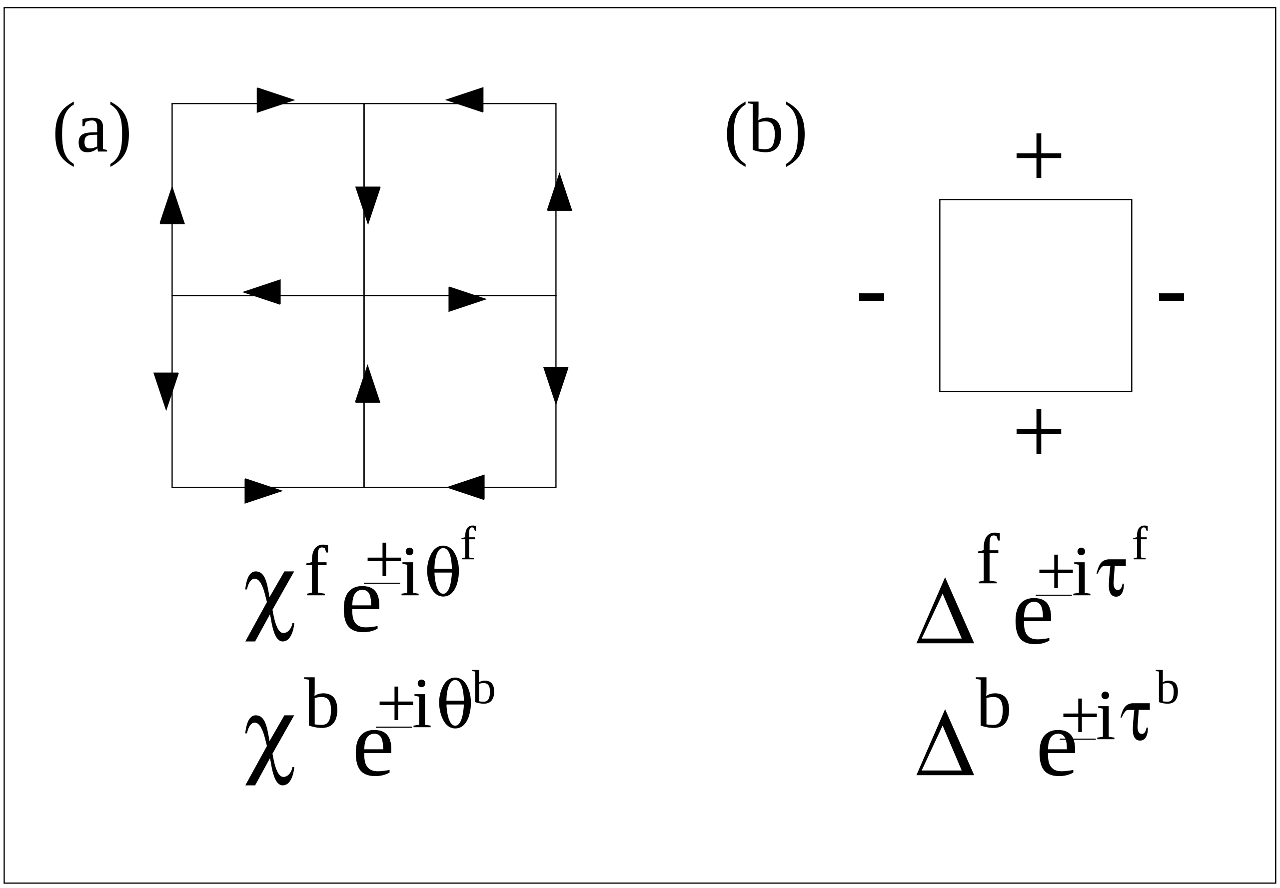
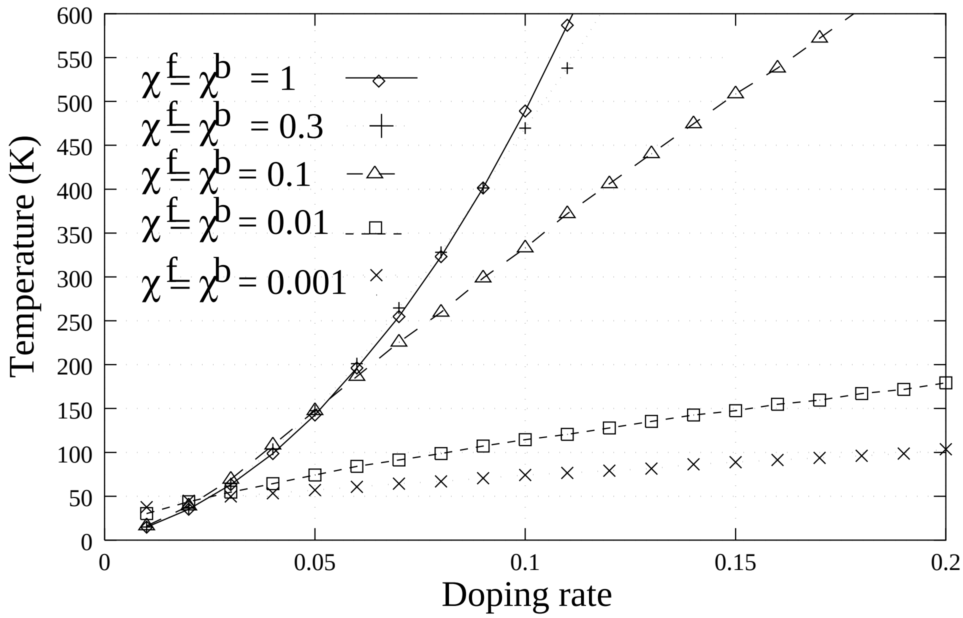


FIG. 1.



Temperature (K)
Doping rate
χ f = χ b = 1
χ f = χ b = 0.3
χ f = χ b = 0.1
χ f = χ b = 0.01
χ f = χ b = 0.001
0
50
100
150
200
250
300
350
400
450
500
550
600
0
0.05
0.1
0.15
0.2

FIG. 2.

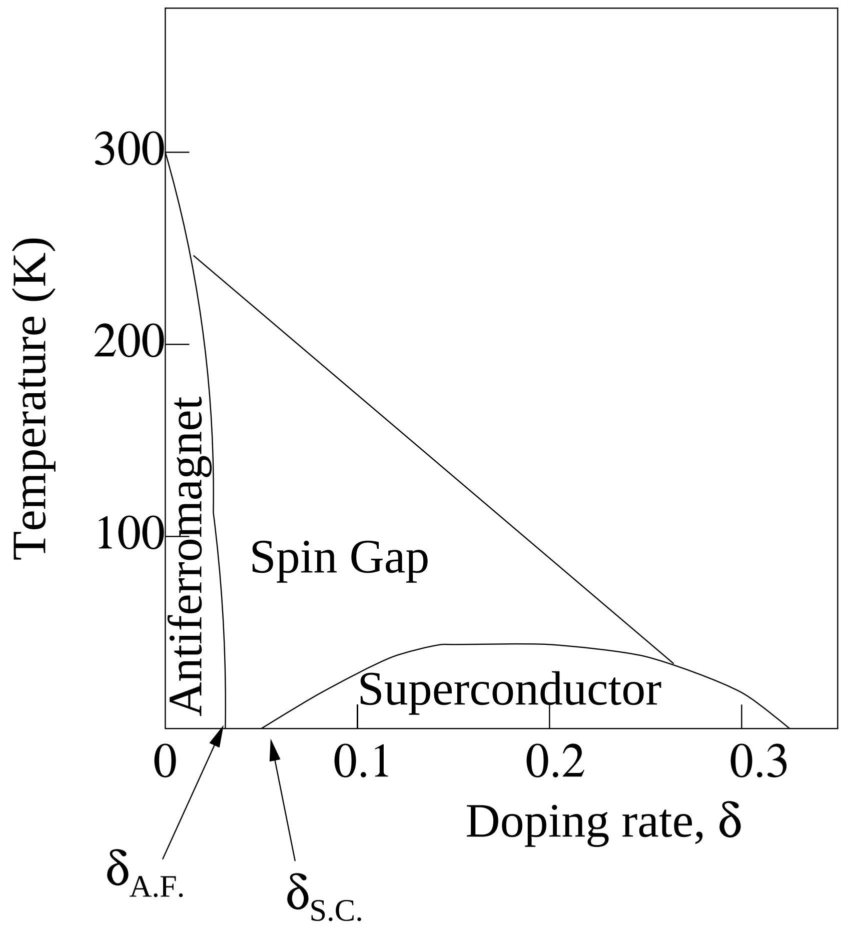

Temperature (K)
300
200
100
Antiferromagnet
Spin Gap
Superconductor
0
0.1
0.2
0.3
Doping rate, δ
δA.F.
δS.C.

FIG. 3.