Interplay of staggered flux phase and *d*-wave superconductivity

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We present a detailed study of the competition and interplay between the staggered flux phase ordering *d*-density wave (DDW) and $d_{x^2-y^2}$ superconductivity within mean field theory. An analytic expression for the temperature dependence of the DDW order parameter is obtained. The strong competition between the two order parameters is demonstrated through their unusual temperature dependencies and its importance in calculating single-particle spectral function has been pointed out. In particular, it is shown that in a perfect square lattice with only nearest-neighbor hopping (t_1), which preserves nesting of the Fermi surface, one of the order parameters is completely inhibited by the other (at a given concentration of hole). In this case the DDW state produces more of a ‘‘real gap’’ rather than a ‘‘pseudogap’’ in the quasiparticle energy. We demonstrate that a finite negative next-nearest-neighbor hopping (t_2) stabilizes the DDW state at underdoping, while very close to the half filling or well inside the underdoped regime, t_2 suppresses DDW order strongly and enhances superconductivity. The actual coexistence between the two orders is established only at finite t_2. The superconducting T_c is always found to be maximum at a doping concentration where the corresponding T_{DDW} goes to zero, the superconducting T_c decreases on further increase of the doping concentration.

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I. INTRODUCTION

The underdoped cuprate superconductors exhibit pseudogap behavior[1] below a characteristic temperature T^*, well above the superconducting transition temperature (T_c). The pseudogap behavior is visualized as a strong suppression of low-frequency spectral weight below T^*. This anomalous phenomenon has been observed in angle-resolved photoemission spectroscopy (ARPES),[2,3] specific-heat,[4] tunneling,[5] NMR,[6] and optical conductivity[7] measurements. A variety of theoretical scenarios has been proposed for the origin of the pseudogap, although no consensus has been achieved so far.

Broadly, these theoretical scenarios may be divided into two categories. One is based on the idea that the pseudogap is due to precursor superconductivity, in which pairing takes place at T^* but achieves coherence only at T_c.[8–14] The other assumes that the pseudogap behavior is related to dynamical fluctuations of some order, such as spin,[15–19] charge, or structural. Some experiments such as ARPES (Refs. 2 and 3) and tunneling[5] show that the normal-state pseudogap has the same angular dependence and magnitude as the superconducting (SC) gap indicating the same symmetry. This makes the SC fluctuation origin of the pseudogap attractive. Recent detailed calculations by Paramekanti *et al.*,[20] reveal that the SC dome is obtained because of the Mott physics at half filling, even though spin pairing is strongest there. Their variational calculation predicts evolution of the system from an undoped resonating valence bond insulator to a *d*-wave superconductor to a Fermi liquid with increasing hole doping. This along with earlier theories qualitatively explains why the doping (x) dependence of T^* has an exactly opposite trend as that of T_c in the low doping regime, even though the two phenomena are believed to be intimately related.

Furthermore, there is some experimental evidence pointing to the existence of superconducting fluctuations like diamagnetic activity above T_c (Ref. 21) and vortexlike excitations in $La_{2-x}Sr_xCuO_4$ indicating fluctuating superfluid density below T^*.[22] The origin of the pseudogap is still controversial. More profoundly, recent detailed investigations of specific-heat, tunneling, NMR, and transport properties[23] strongly indicate that the origin of the pseudogap is from some competing condensation other than superconductivity itself. For example, Zn substitution on Cu is known to suppress SC strongly while such substitution results in *no suppression* of the pseudogap.[23]

The phase diagram of high-temperature cuprate superconductors is very rich. In addition to antiferromagnetism, $d_{x^2-y^2}$ pairing, and charge ordering, staggered orbital antiferromagnetism produced by local circulating currents has joined the list of physical states that might occupy a prominant place in the phase diagram.[24] Physically, these currents alternate in sign from plaquette to plaquette in the copper-oxygen plane and comprise the staggered flux phase. Therefore, the staggered flux phase is also known as the density-wave state having $d_{x^2-y^2}$ symmetry (i.e., DDW) or the *d*-CDW state (the charge-density-wave state with $l=2$). The essential feature of the *d*-CDW state is that staggered orbital magnetic moments (or staggered currents) break parity and time-reversal symmetry by one lattice constant and $\pi/2$ rotations. This new kind of order parameter which is purely imaginary is fundamentally different from the other proposed theories mentioned above. Furthermore, as it is well known that the charge-density wave and superconductivity compete with each other in a strongly correlated system (both of which will have advantage of avoiding Coulomb repulsion due to their d-wave symmetry), a pseudogap arising from a d-density-wave state therefore has immense appeal. Although the debate about the mechanism for the pseudogap is yet to be settled, it is suggested that the essential characteristics of the pseudogap as observed in many recent experiments, including photoemission,[25] tunneling,[26] and muon spin relaxation,[27] can be explained by the DDW model. More recently, the detection of the DDW ordering using impurity resonance has also been proposed.[28] Therefore, if the DDW state is responsible for the pseudogap phase, its effect on the d-wave superconductivity (DSC) must be understood.

In the present paper we study in detail the coexistence of the DDW and DSC within mean-field theory. We show that with decreasing doping (towards optimal doping) the DDW state produces a gap in the single-particle spectrum at around $(\pi,0)$ of the Fermi surface and competes with d-wave pairing, leading to the arrest of the growth of superconductivity in the underdoped regime. This strong competition results in unusual temperature dependencies of the two order parameters. In particular, it is shown that when nesting of the Fermi surface is perfect, as in a square lattice with only nearest-neighbor (nn) hopping (t_1), one of the order parameters is completely inhibited by the other. In fact, the DDW state produces more of a ''real gap'' rather than a ''pseudogap'' in the quasiparticle energy spectrum. We demonstrate that a finite negative next-nearest-neighbor (nnn) hopping (t_2), which is realistic for high-T_c cuprates, stabilizes the DDW state near optimum doping without affecting DSC. On the other hand, t_2 suppresses the DDW strongly and enhances superconductivity close to half filling. The actual coexistence of the two orders is established only at finite t_2. The T_c is always found to be maximum at a doping concentration where the corresponding T_{DDW} (DDW transition temperature) drops to zero and it decreases with further doping.

The layout of the paper is as follows. In Sec. II we briefly discuss the essential features of a DDW phase and obtain analytical expressions for the transition temperature and gap magnitude. In Sec. III we consider the coexistence of the DDW and DSC states at the mean-field level and obtain the coupled gap equations. Section IV discusses the numerical results of the interplay of the DDW and DSC. Concluding remarks are added in Sec. V.

II. DDW STATE

Microscopic Hamiltonians responsible for various DDW states have been discussed in detail by Nayak and his collaborators.[24,16,30] Here we present a phenomenological model for the DDW state with $\vec{Q}=(\pi,\pi)$, and analytically obtain the gap equation and the transition temperature.

The mean-field Hamiltonian for the DDW state is

$$H_{\rm DDW}=\sum_{k,\sigma}^{\rm FBZ}(\epsilon_k-\mu)c_{k,\sigma}^{\dagger}c_{k,\sigma}+\sum_{k,\sigma}^{\rm RBZ}iW_k c_{k,\sigma}^{\dagger}c_{k+Q,\sigma}+\text{H.c.}, \tag{1}$$

where FBZ and RBZ denote the full and reduced Brillouin zones, respectively, $\epsilon_k^{\rm nn}=-2t_1(\cos k_x+\cos k_y)$, and the band energy $\epsilon_k=\epsilon_k^{\rm nn}+\epsilon_k^{\rm nnn}$ with $\epsilon_k^{\rm nn}=-2t_1(\cos k_x+\cos k_y)$ and $\epsilon_k^{\rm nnn}=-4t_2\cos k_x\cos k_y$. W_k is defined as

$$W_k=W_0 f_k=i\sum_{k'}V_{k,k'}^{\rm CDW}\langle c_{k'+Q,\sigma}^{\dagger}c_{k',\sigma}\rangle, \tag{2}$$

where $f_k=\cos k_x-\cos k_y$ describes the d-wave symmetry of the order parameter. Here $V_{k,k'}^{\rm CDW}$ is the interaction term in the relevant channel and has been assumed to have the separable form $V_0^{\rm CDW}f_k f_{k'}$. In order for Hamiltonian (1) to be Hermitian, the order parameter (OP) iW_k of the d-CDW state must be purely imaginary, which follows from the property $W_k={}^-W_{k+Q}$.

The Hamiltonian in Eq. (1) may be rewritten as

$$H_{\rm DDW}=\sum_{k,\sigma}\Psi_{k,\sigma}^{\dagger}\hat{H}(k)\Psi_{k,\sigma}$$

with

$$\hat{H}(k)=\begin{pmatrix}\epsilon_k^{\rm nn}+\epsilon_k^{\rm nnn}-\mu & iW_k\\ -iW_k & -(\epsilon_k^{\rm nn}-\epsilon_k^{\rm nnn}+\mu)\end{pmatrix} \tag{3}$$

and $\Psi_{k,\sigma}^{\dagger}=(c_{k,\sigma}^{\dagger}\ c_{k+Q,\sigma}^{\dagger})$. Here nesting of the Fermi surface (FS) holds only for a part of the FS, namely, $\epsilon_k^{\rm nn}=-\epsilon_{k+Q}^{\rm nn}$.

The eigenvalues of the $\hat{H}$ yield the quasiparticle energy spectrum of the DDW state, given by $E_k^{c(v)}=\epsilon_k^{\rm nnn}-\mu\pm E_k^0$ where $E_k^0=\sqrt{\epsilon_k^{\rm nn^2}+W_k^2}$. Only part of the band energy $\epsilon_k^{\rm nn}$ and hence the FS is gapped. So this is a metallic DDW state with a pseudogap.

For convenience we find a new basis set $\Phi_{k,\sigma}^{\dagger}=(\gamma_{k,\sigma}^{c^{\dagger}}\ \gamma_{k,\sigma}^{v^{\dagger}})$ through a unitary transformation such that $\hat{H}(k)\Psi_k=E_k\Psi_k=E_kUU^{-1}\Psi_kUU^{-1}=E_kU\Phi_kU^{-1}$ which diagonalizes the Hamiltonian (1) completely, $\hat{H}_{\rm diag}(k)\Phi_k=E_k\Phi_k$, where $\Phi_k=U^{-1}\Psi_kU$ and is related to Ψ_k as follows,

$$\Psi_k=\begin{pmatrix}iu_k & v_k\\ v_k & iu_k\end{pmatrix}\Phi_k, \tag{4}$$

where the d-CDW coherence factors, $u_k(v_k)=\frac{1}{\sqrt{2}}[1\pm(\epsilon_k^{\rm nn}/E_k^0)]^{1/2}$. With the help of canonical transformation (4) on Eq. (3) the mean-field DDW Hamiltonian reduces to

$$H_{\rm DDW}=\sum_{k,\sigma}E_k^c\gamma_{k,\sigma}^{c^{\dagger}}\gamma_{k,\sigma}^c+E_k^v\gamma_{k,\sigma}^{v^{\dagger}}\gamma_{k,\sigma}^v. \tag{5}$$

Now it is very convenient to calculate the expectation value on the right-hand side of Eq. (2) using the transformation (4) and the Hamiltonian (5). This leads to the self-consistent gap equation for the DDW state,

$$1=\frac{V_0^{\rm CDW}}{2}\sum_k\frac{f_k^2}{E_k^0}\left[\tanh\left(\frac{\beta E_k^c}{2}\right)-\tanh\left(\frac{\beta E_k^v}{2}\right)\right]. \tag{6}$$

In the limit of $t_2=0.0$ and at half filling ($\mu=0$), $E_k^c=-E_k^v=E_k^0$. The DDW gap equation Eq. (6) takes the form

$$1=V_0^{\mathrm{CDW}}\sum_k \frac{f_k^2}{E_k^0}\tanh\left(\frac{\beta E_k^0}{2}\right). \tag{7}$$

Note the formal similarity of this gap equation for the DDW with a simple BCS *d*-wave gap equation. At $T=0$, the above equation can also be written as

$$\begin{aligned}1&=V_0^{\mathrm{CDW}}\sum_{k,\phi}\frac{\cos^2 2\phi}{\sqrt{\epsilon^2+W_0^2\cos^2 2\phi}}\\&=V_0^{\mathrm{CDW}}N(\epsilon_F)\int_{-\omega_c/2}^{\omega_c/2}d\epsilon\int_0^{2\pi}\frac{d\phi}{2\pi}\frac{\cos^2 2\phi}{\sqrt{\epsilon^2+W_0^2\cos^2 2\phi}},\end{aligned} \tag{8}$$

where $\phi=\tan^{-1}(k_y/k_x)$ and $N(\epsilon_F)$ is the density of states at the Fermi level. Equation (8) can easily be used to find the zero-temperature magnitude of the DDW gap and the corresponding transition temperature (T_{DDW}) as follows,

$$W_0=\frac{2\omega_c}{\sqrt{e}}\exp\left(-\frac{1}{N(\epsilon_F)V_0^{\mathrm{CDW}}}\right) \tag{9}$$

and

$$T_{\mathrm{DDW}}=\frac{\gamma\omega_c}{\pi}\exp\left(-\frac{1}{N(\epsilon_F)V_0^{\mathrm{CDW}}}\right), \tag{10}$$

where $\ln\gamma\approx0.577$ is the Euler's constant. The ratio of the DDW gap and the transition temperature is $2W_0/k_BT_{\mathrm{DDW}}\sim4.3$. One can also get analytic expressions for the temperature-dependent DDW gap following standard expansions at $T\ll T_{\mathrm{CDW}}$ and $(T_{\mathrm{CDW}}-T)\ll T_{\mathrm{CDW}}$,[31] as below:

$$\frac{\Delta_{\mathrm{CDW}}(T)}{\Delta_{\mathrm{CDW}}(0)}=\left[1-0.37\left(\frac{T}{T_{\mathrm{CDW}}}\right)^3\right];\quad\left(\frac{T}{T_{\mathrm{CDW}}}\right)\ll1 \tag{11}$$

and

$$\frac{\Delta_{\mathrm{CDW}}(T)}{\Delta_{\mathrm{CDW}}(0)}=1.65\sqrt{1-\left(\frac{T}{T_{\mathrm{CDW}}}\right)};\quad 1-\frac{T}{T_{\mathrm{CDW}}}\ll1. \tag{12}$$

In deriving Eqs. (9)–(12) the density of states (DOS) around the Fermi level $N(E_F)$ is assumed to be constant. Based on these approximate expressions at the two extreme regions of temperatures, extrapolating (fitting) them and with the help of numerical calculations, we arrive at an analytical expression for the DDW gap at any temperature:

$$\Delta_{\mathrm{CDW}}(T)=\Delta_{\mathrm{CDW}}(0)\left[1-0.95\left(\frac{T}{T_{\mathrm{CDW}}}\right)^{3.5}\right]^{0.6}. \tag{13}$$

We emphasize that this expression is also valid for pure *d*-wave superconductors (T_{CDW} would be replaced by T_c). Such an analytic equation, to our knowledge, has not been obtained so far and should be checked by others. We shall show that this analytic equation obeys all our numerical data.

Since nesting is not perfect due to finite doping or t_2 and other higher-order hoppings present in high-T_c systems (our formalism is valid for any order of hoppings; non-nested band energies may be included in $\epsilon_k^{\mathrm{nnn}}$), fluctuations of the DDW state will be very strong. In fact, the maximum frequency for the amplitude (collective-) mode fluctuations of the DDW gap will be $\Omega=2W_k$, as discussed in more detail in Ref. 29. Therefore, given the realistic situation in high-T_c systems, the system will have a strongly fluctuating DDW state, which may mediate *d*-wave superconductivity. In this paper our main aim, however, is to understand the physical situation due to interplay of the DDW and DSC.

III. COEXISTENCE OF THE DDW AND DSC

In this section we show that there is a strong interplay between the staggered flux phase and *d*-wave superconductivity (DSC) which leads to an interesting phase diagram. Coexistence of the pseudogap (DDW) with superconductivity (DSC) (below T_c) is consistent with experimental findings and we demonstrate the same only in the presence of finite t_2. The microscopic mean-field Hamiltonian appropriate for the coexistence of DDW and DSC states is given as

$$\begin{aligned}H=&\sum_{k,\sigma}^{\mathrm{FBZ}}(\epsilon_k^{\mathrm{nn}}+\epsilon_k^{\mathrm{nnn}}-\mu)c_{k,\sigma}^\dagger c_{k,\sigma}+\sum_{k,\sigma}^{\mathrm{RBZ}} iW_kc_{k,\sigma}^\dagger c_{k+Q,\sigma}+\mathrm{H.c.}\\&+\sum_k^{\mathrm{RBZ}}(\Delta_kc_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger-\Delta_kc_{k+Q,\uparrow}^\dagger c_{-k-Q,\downarrow}^\dagger+\mathrm{H.c.}).\end{aligned} \tag{14}$$

Δ_k is the superconducting order parameter with $d_{x^2-y^2}$ symmetry having the form $\Delta_k=\Delta_0f_k$, and therefore $\Delta_{k+Q}=-\Delta_k$. The Hamiltonian (14) can be written with the help of a four-component Nambu operator $\Psi_k^\dagger=(c_{k\uparrow}^\dagger\ c_{k+Q\uparrow}^\dagger\ c_{-k\downarrow}\ c_{-k-Q\downarrow})$ as

$$H=\sum_k\Psi_k^\dagger\hat{H}(k)\Psi_k, \tag{15}$$

where

$$\hat{H}=\begin{pmatrix}\epsilon^+-\mu & iW_k & \Delta_k & 0\\ -iW_k & -(\epsilon^-+\mu) & 0 & -\Delta_k\\ \Delta_k & 0 & -(\epsilon^+-\mu) & iW_k\\ 0 & -\Delta_k & -iW_k & (\epsilon^-+\mu)\end{pmatrix}, \tag{16}$$

where $\epsilon^\pm=\epsilon_k^{\mathrm{nn}}\pm\epsilon_k^{\mathrm{nnn}}$. The eigenvalues of the above matrix, describing the quasiparticle energy spectrum of the coexistence phase, are given as $E_{1,2}(k)=\pm\sqrt{\Delta_k^2+(E_k^0\pm\epsilon_k^{\mathrm{nnn}}-\mu)^2}$, where $E_k^0=\sqrt{\epsilon_k^{nn^2}+W_k^2}$. The *d*-wave superconducting order parameter is defined as

$$\Delta_k=\sum_{k'}V_{k,k'}^{\mathrm{SC}}\langle c_{-k\downarrow}c_{k\uparrow}\rangle, \tag{17}$$

where $V^{\rm SC}_{k,k'}=V^{\rm SC}_0 f_k f_{k'}$. Following the same procedure as in an earlier section we diagonalize the Hamiltonian (14) as follows:

$$H=\sum_k E_1(k)(\alpha_k^\dagger\alpha_k-\beta_k^\dagger\beta_k)+E_2(k)(\gamma_k^\dagger\gamma_k-\delta_k^\dagger\delta_k). \tag{18}$$

The necessary canonical transformation is obtained to be

$$\Psi_k=\begin{pmatrix} -iu_k\tilde{u}_k & iu_k\tilde{v}_k & -iv_k\tilde{u}'_k & iv_k\tilde{v}'_k \\ -v_k\tilde{u}_k & v_k\tilde{v}_k & u_k\tilde{u}'_k & -u_k\tilde{v}'_k \\ -iu_k\tilde{v}_k & -iu_k\tilde{u}_k & iv_k\tilde{v}'_k & iv_k\tilde{u}'_k \\ v_k\tilde{v}_k & v_k\tilde{u}_k & u_k\tilde{v}'_k & u_k\tilde{u}'_k \end{pmatrix}\times\Phi_k, \tag{19}$$

where $\Phi_k^\dagger=(\alpha_k^\dagger\ \beta_k^\dagger\ \gamma_k\ \delta_k)$ and the superconducting coherence factors are given by $\tilde{u}_k(\tilde{u}'_k)=(1/\sqrt{2})[1+(E_k^0\pm\epsilon_k^{\rm nnn}\mp\mu)/E_{1(2)}]^{1/2}$ and $\tilde{v}_k(\tilde{v}'_k)=(1/\sqrt{2})[1-(E_k^0\pm\epsilon_k^{\rm nnn}\mp\mu)/E_{1(2)}]^{1/2}$. Now, we calculate the averages in Eq. (17) as well as that in Eq. (2) using Eqs. (15), (18), and (19). This gives rise to the coupled integral gap equations for the coexistence phase of DDW and *d*-wave superconductivity as given below,

$$1=V_0^{\rm CDW}\sum_k\frac{f_k^2}{E_k^0}\left\{\frac{E_k^0+\epsilon_k^{\rm nnn}-\mu(T)}{2E_1(k)}\tanh\frac{\beta E_1(k)}{2}+\frac{E_k^0-\epsilon_k^{\rm nnn}+\mu(T)}{2E_2(k)}\tanh\frac{\beta E_2(k)}{2}\right\} \tag{20}$$

and

$$1=V_0^{\rm SC}\sum_k f_k^2\left[\frac{\tanh\frac{\beta E_1(k)}{2}}{2E_1(k)}+\frac{\tanh\frac{\beta E_2(k)}{2}}{2E_2(k)}\right]. \tag{21}$$

It may be noted that Eq. (20) reproduces Eq. (6) in the limit $\Delta_k\to0$, with proper signs taken into account. Similarly, in the limit of $W_k\to0$, Eq. (21) reduces to the simple BCS gap equation for DSC. The band filling n can be varied by tuning the chemical potential μ and may be calculated through the relation $n=1/N\Sigma_{k,\sigma}\langle c^\dagger_{k,\sigma}c_{k,\sigma}\rangle$. Using Eqs. (18) and (19) we obtain

$$n=\frac{1}{N}\sum_k\left\{1-\frac{E_k^0+\epsilon_k^{\rm nnn}-\mu(T)}{2E_1(k)}\tanh\frac{\beta E_1(k)}{2}+\frac{E_k^0-\epsilon_k^{\rm nnn}+\mu(T)}{2E_2(k)}\tanh\frac{\beta E_2(k)}{2}\right\}. \tag{22}$$

In the limit of $t_2=0$ (i.e, $\epsilon_k^{\rm nnn}=0$), at half filling ($\mu=0$) $E_1=E_2$ and n reduces to unity, as it should.

Now, the study of interplay of the staggered flux phase (or DDW state) with *d*-wave superconductivity amounts to solving the coupled Eqs. (20)–(22) self-consistently corresponding to the three functions $W_k\equiv W_k(W_k,\Delta_k,\mu(T))$, $\Delta_k\equiv\Delta_k(W_k,\Delta_k,\mu(T))$, and $\mu(T)\equiv\mu(W_k,\Delta_k,\mu)$. It should be noted that in this process the temperature variation of the chemical potential must be incorporated (see below for further discussion). The interaction strengths $V_0^{\rm CDW}$ and $V_0^{\rm SC}$ are chosen as 0.06 eV and 0.05 eV, respectively. The energy cutoffs around the Fermi surface over which these interaction strengths are effective are chosen as 0.08 eV and 0.06 eV, respectively. At half filling and $t_2=0$ these parameters give $T_{\rm CDW}$ of 180 K in the absence of superconductivity and T_c of around 110 K in the absence of the DDW. These parameter values are chosen so that maximum interplay between the two orders takes place, and the values are kept fixed for all the calculations in this paper. Slight changes in the cutoff frequencies do not correspond to any qualitative changes in our results. We notice that U(1) mean-field theory of the *t*-*J* model gives rise to $V^{\rm CDW}=0.5J$ and $V^{\rm SC}=J$, however, no bulk DDW state was found in this model.[32] We actually found an interesting regime of interplay only when $V_0^{\rm CDW}>V_0^{\rm SC}$. We discuss our numerical solutions of the above equations in the next section.

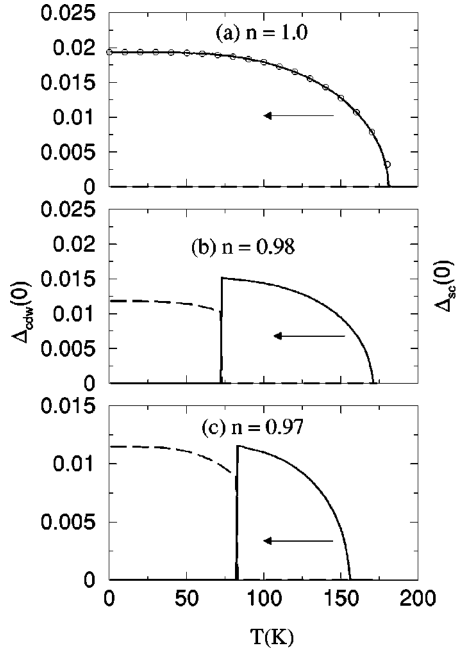

FIG. 1. Temperature variations of the DDW (solid lines) and DSC order (dashed lines) parameters in the absence of next-nearest-neighbor hopping $t_2=0.0$ for various values of band filling (n). Note the peculiar temperature dependence of the DSC in (b) and (c) compared to standard second-order phase transitions. We use notations $\Delta_{CDW}(k)=\Delta_{CDW}(0)f_k$ and $\Delta_{SC}(k)=\Delta_{SC}(0)f_k$.

IV. RESULTS AND DISCUSSIONS

A. $t_2=0$

In Fig. 1 we present the temperature dependence of the DDW and DSC energy gaps for various band fillings in the absence of t_2. In this panel of figures thick solid lines correspond to the DDW gap and long-dashed lines to the DSC

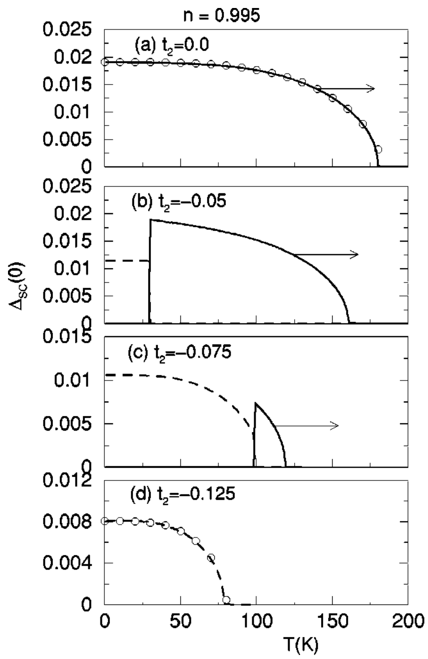

FIG. 2. Temperature dependencies of the DSC (thick dashed lines) and the DDW (thick solid lines) gap parameters in the presence of t_2 at 0.5% doping. It is worth noting that for smaller values of t_2 the DDW transition temperatures are suppressed whereas the SC correlations are enhanced. The trend changes at $t_2 = -0.125t_1$.

gap. Energy-gap scales are in eV whereas temperatures are in Kelvin. In the very low doping regime or very close to the half filling no DSC is found whereas no DDW state is found above 4% of doping.

Due to perfect nesting at half filling of the square lattice there will be a strong instability of the FS due to DDW formation and hence there will be no carriers available for pairing resulting in the vanishing of the DSC gap [see Fig. 1(a)]. The scenario changes abruptly as one dopes the system and nesting of the FS is violated; this results in very rapid suppression of the DDW gap with doping. In competition, thereby, the DSC state starts appearing as one dopes the system. More quantitatively, a small doping of about 3.5% reduces the transition temperature for the DDW state by about 35 K (not shown in the figure), whereas the DSC transition temperature increases by 100 K. Thus we see that each order inhibits the other very strongly.

In addition to the strong tendency towards DDW formation at half filling, the *d*-wave SC state is also strongly favored due to the Van Hove singularity in the normal-state DOS. This results in a strong competition between the two orders near half filling. In fact, this competition is so strong that even a smaller DSC gap completely suppresses a larger DDW gap [see Figs. 1(b) and 1(c), and also Fig. 2(b)]. Thus, with doping the CDW gap decreases sharply whereas the SC gap and its transition temperature increases. The highest T_c is obtained when the DDW gap just vanishes. Further increase in hole doping reduces the T_c.

B. $t_2 \neq 0$

In Fig. 2 we have plotted the temperature dependence of the DDW and DSC gaps for a fixed doping concentration (near half-filling) and several values of t_2, in order to study the role of second-neighbor hopping on the interplay between the DDW and DSC orders. It is worth mentioning at this stage that it was found from ARPES data on $Bi_2Sr_2CaCu_2O_8$ at optimal doping[33] that the next-nearest-neighbor hopping is negative with respect to the nearest-neighbor hopping, and can be as large as $0.25t_1$.[33] Therefore, our choice of values and sign of t_2 is in accordance with these observations. General features of Fig. 1, i.e., existence of only DSC at lower temperatures and only DDW at higher temperatures, are retained in Fig. 2 as well. As t_2 increases, the DDW state is strongly suppressed whereas the DSC phase is strongly favored; a t_2 as small as $0.125t_1$ completely suppresses the DDW state with $T_{\mathrm{DDW}} = 180$ K [cf. Figs. 2(a) and 2(d)]. On the other hand, such a small change in t_2 can strongly stabilize the DSC by setting a T_c as high as 100 K from 0 K [cf. Figs. 2(a) and 2(c)]. Maximum T_c is found only when DDW order just vanishes [cf. Fig. 2(c) and Fig. 2(d)]. This feature is found to be universal at the optimum doping (at which maximum T_c occurs).

Therefore, in these figures we have only one of the order parameters surviving—the DSC gap at lower temperatures and the DDW gap at higher temperatures. This feature is very important for calculation of the single-particle spectral function, etc. Although an effective gap $\sqrt{W_k^2 + \Delta_k^2}$ appears in the quasiparticle energy spectrum, either W_k or Δ_k survives. Another feature to be noticed is that the temperature variations of the DSC gaps are quite unusual in the sense that the gap vanishes suddenly almost like a first-order phase transition. Furthermore, because of this strange interplay between the DDW and the SC states, the BCS ratio, $2\Delta^{max}/k_B T_c$, is much larger compared to the standard weak-coupling value of 4.3 (for *d*-wave superconductors) at small doping which is typical of high-T_c cuprates. Therefore, interplay of the DDW with DSC can make fundamental modifications to the temperature dependencies of each other.

These results described above may be understood qualitatively within the discussions on the loss of nesting due to t_2 and its effect on the DDW state in connection with Fig. 1. However, those arguments are valid only close to half filling: introduction of t_2 causes loss of nesting and damages the DDW very strongly and thus in competition SC enhances. Therefore, t_2 enhances the possibility of SC appearing close to half filling. We should mention that no antiferromagnetic order is considered in our self-consistent model calculation, therefore the possibility of SC close to half filling appears. Finally, we display the analytical Eq. (13) for a *d*-wave gap in Figs. 1(a), 2(a), and 2(d) with circular points. This establishes that the (empirical) analytical expression obtained in Eq. (13) closely represents the exact result for any *d*-wave gap.

In Fig. 3 we present the same data as that in Fig. 2 but at a higher doping concentration of 7%. Here we show that exactly the opposite happens to the DDW compared to that in Fig. 2. In Fig. 3(a) there was no DDW when $t_2 = 0.0$, which appears with a $T_{\mathrm{DDW}} \approx 125$ K for a small increase of $t_2 = -0.075t_1$ [see Fig. 3(b)] although the SC gap and T_c remain almost unaltered (increase only slightly). Even

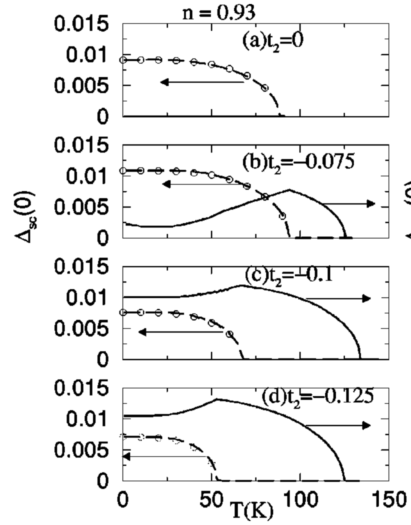

FIG. 3. Thermal variations of the DSC and the DDW gap parameters in the presence of t_2 at 7% doping. Notations are same as that in Fig. 2. Note a different role of t_2 than that in Fig. 2: t_2 stabilizes the DDW as well as its coexistence with DSC. The arrest of the growth of the DDW gap with the appearance of DSC is worth noting [e.g., see (b)–(d)].

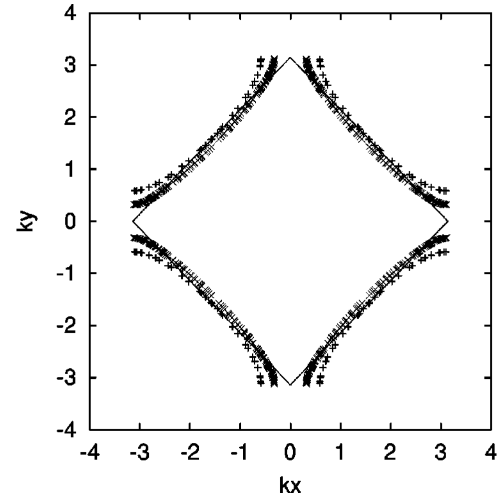

FIG. 4. Noninteracting FS for various dopings (μ) and (t_2). The perfect square FS, represented by the thin solid line corresponding to $t_2=0$ at half filling, has a large nested area. The FS curve with cross (less dense) symbols represents $\mu=0$ and $t_2=-0.1t$. Now when μ is decreased to -0.07 (and hence with increased doping) a large amount of FS nesting is recovered (see the densest curve with the small parallel bar).

though the SC gap is larger compared to that of the DDW, the DDW gap is not completely suppressed and the two orders coexist. With further increase in t_2 to $-.1t_1$ or $-.125t_1$ the DDW amplitude is enhanced further whereas the DSC is suppressed. However, a further increase in t_2 again suppresses the DDW and hence enhances SC. These behaviors have important bearings related to the nesting of the FS as discussed below.

We also emphasize that we see the actual coexistence between the two orders for the first time in Figs. 3(b)–3(d). Here both the order parameters *coexist*, although the appearance of superconductivity arrests the growth of the DDW with decreasing temperature. Therefore, t_2 at higher doping stabilizes the DDW state. This again can be understood in terms of FS nesting.

Interestingly, the thermal variation of the DSC is exactly governed by the analytical Eq. (13), *even* in the coexistent phase. This is shown by the circular points over the dashed lines. Therefore, the DSC can coexist *independently* with the DDW phase. This is further established from the fact that the circular points obtained from Eq. (13) exactly overlap with the numerical data which are self-consistent solutions of the coupled Eqs. (20)–(22). Hence Eq. (13) is the analytical solution for any d-wave OP at finite temperature.

In Fig. 4 we present the noninteracting FS's. This successfully demonstrates that while doping destroys the FS nesting, t_2 brings back a large amount of nesting at higher doping. Thereby, DDW order is enhanced. In Fig. 4(a), the solid perfect square presents the FS at half filling in the absence of the next-nearest-neighbor hopping (t_2). In Fig. 4(b), the less dense cross-symbol curve represents the FS for $t_2=-0.1t_1$ and $\mu=0$ [this therefore corresponds to going away from half filling in contrast to Fig. 4(a)]. In Fig. 4(c), the dense curve with thin parallel bar symbols corresponds to the FS with the same value of t_2 as that in the case of Fig. 4(b) but with $\mu=-0.07$. It can be seen that the "gap" opened around the high-symmetry (π,0) points (corners, rather) in Fig. 4(b) reduces in the case of Fig. 4(c), reproducing more regions of flat Fermi line segments that can be translated to fall on the other side of the FS and hence FS nesting is enhanced. However, on further increase of chemical potential (μ) and hence doping, the "gaps" increase again (not shown in the figure for clarity) and separate into four different branches of parabolic segments with less nesting. This behavior of the FS topology has an important influence on the coexistence phase of the DDW and DSC, in the sense that in the region $V^{\mathrm{CDW}}>V^{\mathrm{SC}}$ more nesting will favor the DDW and hence in competition DSC will be suppressed and vice versa. These features are obvious from Figs. 2 and 3.

It will be interesting to study how the energy gaps behave for different dopings at a fixed t_2. This has been displayed in Fig. 5; for a fixed $t_2=-0.1t_1$ the temperature dependencies of the order parameters are plotted for various band fillings. For $n=0.97$ no coexistence is found and at lower temperatures DSC order is strong enough to suppress the DDW. As the system is further doped the superconductivity is suppressed and the DDW state extends all the way from low to high temperature, coexisting with the superconductivity. More importantly, the T_{DDW} remains almost constant until $n=0.93$ whereas the DSC state continues to grow within the DDW phase at lower temperatures causing only a small suppression in the amplitude of the DDW gap [see Figs. 5(b)–5(d)]. Interestingly, even a larger SC gap than that of the DDW does not completely suppress the DDW at lower temperatures [cf. Fig. 5(e)] and a true coexistence between them is established. This behavior may be contrasted with those in Figs. 1 and 2.

We will draw an approximate phase diagram based on these discussions of Figs. 1–5. Before that, we present the

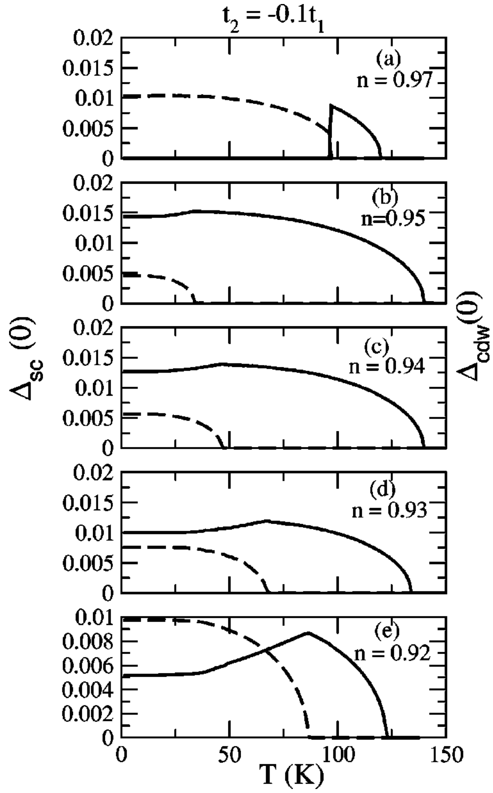

FIG. 5. Effect of doping on the temperature dependencies of the DDW (solid line) and the DSC (dashed line) order parameters for a fixed $t_2 = -0.1t_1$.

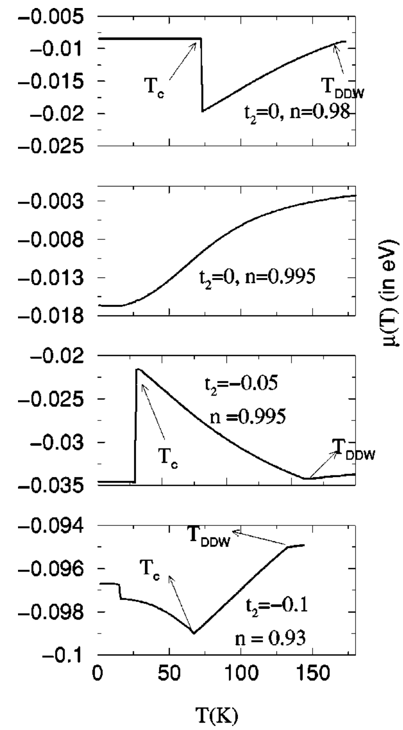

FIG. 6. Strong temperature dependence of the chemical potential (μ). Abrupt changes in μ with temperature correspond to transition points (see also Figs. 1–3) for comparison.

temperature dependence $[\mu(T)]$ of the chemical potential in Fig. 6. The top two figures correspond to situations of Fig. 1(a) and Fig. 2(a) while the remaining two correspond to Figs. 2(b) and 3(c). These drastic changes of μ with temperature have a strong influence, and are properly taken care of within the self-consistent solution of the order parameters. The sudden changes in μ correspond to the SC and DDW transition points as observed in Figs. 1(b), 1(c), 2(b), and 2(c).

The phase diagram shown in Fig. 7 comprises transition temperatures (T_{DDW} for DDW and T_c for DSC) as a function of doping (δ). In Fig. 7(a) no coexistence is found, i.e, below optimum doping only the DDW order exists at higher temperatures whereas only DSC exists at lower temperatures. For quite a different set of parameters we do not expect any qualitative changes to the phase diagram but one *may* have a coexistence phase within a very thin doping region, $\delta = 0.025$–0.03. However, we did not find any coexistence phase within the set of parameters used, although the two orders influence very strongly each other (namely, the DDW order would not have been suppressed if the DSC were not present at lower temperatures). By a coexistence phase we mean a region of temperature and doping where magnitudes of both the order parameters are nonzero, such as, for example, the case in Figs. 3(b) and 3(c), but not the case in Fig. 5(a) or Fig. 1. The highest T_c at optimum doping occurs where the DDW vanishes. As t_2 is increased the maximum of the DDW shifts away from half filling to higher dopings. For $t_2 = -0.05t_1$ [Fig. 7(b)] the DDW order is finite but weaker

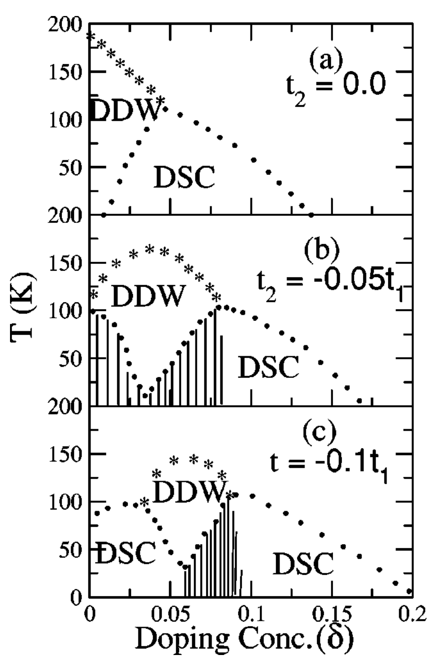

FIG. 7. Phase diagram of the coexistent DDW-DSC for various t_2; transition temperatures T_{DDW} (T_c) are plotted as a function of doping concentration, δ. The coexistence phase extends for higher values of t_2 and the optimum doping shifts to higher values. The shaded region by vertical lines indicates the coexistence phase.

than that in Fig. 7(a) and coexists with DSC represented by the shaded regions. At finite t_2 maximum nesting of the FS is not at half filling but at some other higher doping, thereby the maximum of the DDW ordering correspondingly occurs at that doping. Therefore, as the system is doped away from half filling, the DDW order enhances and the DSC diminishes, and at around $\delta = 0.04$, the DDW attains its maximum whereas the DSC is almost completely suppressed. For doping beyond 0.04, a similar trend to that of Fig. 7(a) is obtained, except that both the orders coexist for a substantial region of doping. The optimum doping where maximum T_c occurs continues to shift to higher values with increasing t_2, however, the maximum T_c does not change much. Also, the total superconducting region enlarges with t_2. At sufficiently large t_2 ($=-0.1t_1$) [Fig. 7(c)], the DDW order at half filling becomes weak enough to be completely suppressed in completion with DSC. Thus, at very close to half filling the DSC prevails alone and this trend continues until slightly more than 5% of doping, and then the coexistence phase establishes.

V. CONCLUSION

We have made a detailed study of the interplay between the DDW and *d*-wave superconductivity. Strong influence and interplay between these ordered phases has been established through their temperature dependencies and detailed study of the phase diagrams reveals its resemblance to that of the high-T_c cuprates. The possibility of either superconductivity or the DDW at half filling appears in the present model as the antiferromagnetic order has not been taken into account in our self-consistent calculation. We have successfully established that a negative next-nearest-neighbor hopping stabilizes the coexistence phase of the two orders. In the absence of next-nearest-neighbor hopping the DDW order appears as a *regular* "real gap" in the energy excitation spectrum, and the resulting coexistence phase becomes almost impossible. In the presence of t_2, a large amount of nesting may be retained at higher doping resulting in enhanced DDW order and thereby opening the possibility for coexistence of the two orders.

We pointed out the importance of this self-consistent calculation for a single-particle spectral function. The spin-spin correlation function $S(Q,\omega)$ at $Q=(\pi,\pi)$ will have a peak near about $\omega = 2\sqrt{W_0^2+\Delta_0^2}$ because the spectral function sum will have restriction of $\delta[\omega - E_1(k) - E_2(k)]$. (At half filling the peak should exactly be at $2\sqrt{W_0^2+\Delta_0^2}$). Therefore, the peak position as well as its strength will strongly depend on doping (and hence on μ) and temperature as governed by the phase diagram (only in restricted cases are both W_0 and Δ_0 nonzero). In some cases, the peak will be governed either by the DSC or DDW depending on the temperature even at a given doping concentration [see Fig. 7(a)]. Similarly, a large number of physical properties that depends on the temperature dependence of the order parameter (for example, specific heat) will strongly be influenced. If DDW order is indeed cause for the pseudogap of the cuprates then the normal state of the cuprates should show a peak/hump in the specific heat at T_{DDW}. In other words, in contrast to the superconducting phase fluctuation scenario of the pseudogap,[14] the DDW phase involves an "extra" thermodynamic phase transition and therefore will be signaled by the corresponding thermodynamic quantities. In particular, if the pseudogap is due to strongly fluctuating but nonvanishing DDW order, a clear signature due to such a phase transition (e.g, a discontinuity in the specific heat) may not be seen experimentally. A large number of experimental properties of the cuprates is consistent with the presence of DDW order in the underdoped cuprates are discussed in detail in Ref. 24. This paper gives the actual behavior of the DDW and the DSC from which a large number of physical properties can be calculated. Furthermore, we have shown that the DDW phase has the correct T^* vs δ behavior. Therefore, given the fact that there are other possible routes from an extra competing condensation scenario that would lead to the pseudogap, the possibility of the DDW as a candidate has been strengthened further. An unique feature of the DDW state is the broken time-reversal and translational symmetries. Therefore, this should be observable, e.g, in neutron scattering the DDW state should have a Bragg signal at the antiferromagnetic wave vector. However, its moment direction, temperature dependence, and Bragg intensities will certainly make a difference between an antiferromagnet and a DDW.[34] Furthermore, since the DDW state breaks time-reversal symmetry, a left circularly polarized light (beam) would produce a photocurrent different from that produced by a right circularly polarized light.

As a word of caution, we would like to mention that the underdoped cuprates have a short coherence length and the phase stiffness is small with small superfluid density. Therefore, phase fluctuations in the underdoped regime are very important and would be considered in future works.

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[1] T. Timusk and B. Statt, Rep. Prog. Phys. **62**, 61 (1999).

[2] H. Ding, T. Yokoya, J.C. Campuzano, T. Takahashi, M. Randeria, M.R. Norman, T. Mochiku, K. Kadowaki, and J. Giapintzakis, Nature (London) **382**, 51 (1996).

[3] A.G. Loeser, Z.-X. Shen, D.S. Dessau, D.S. Marshall, C.H. Park, P. Fournier, and A. Kapitulnik, Science **273**, 325 (1996).

[4] J.W. Loram, K.A. Mirza, J.R. Cooper, and W.Y. Liang, Phys. Rev. Lett. **71**, 1740 (1993).

[5] Ch. Renner, B. Revaz, J.-Y. Genoud, K. Kadowaki, and O. Fisher, Phys. Rev. Lett. **80**, 149 (1998).

[6] M. Takigawa, A.P. Reyes, P.C. Hammel, J.D. Thompson, R.H. Heffner, Z. Fisk, and K.C. Ott, Phys. Rev. B **43**, 247 (1991).

[7] C.C. Homes, T. Timusk, R. Liang, D.A. Bonn, and W.N. Hardy, Phys. Rev. Lett. **71**, 1645 (1993).
[8] V.J. Emery and S.A. Kivelson, Nature (London) **374**, 434 (1995).
[9] R. Micnas, M.H. Pedersen, S. Schafroth, T. Schneider, J.J. Rodrguez-Nez, and H. Beck, Phys. Rev. B **52**, 16223 (1995).
[10] J. Ranninger and J.M. Robin, Phys. Rev. B **53**, R11961 (1996).
[11] M. Randeria, Ji-Min Duan, and Lih-Yir Shieh, Phys. Rev. Lett. **62**, 981 (1989).
[12] T.D. Lee, Nature (London) **330**, 460 (1987).
[13] V.B. Geshkenbein, L.B. Ioffe, and A.I. Larkin, Phys. Rev. B **55**, 3173 (1997).
[14] For a discussion of phase-fluctuation models in *d*-wave superconductors, see A. Paramekanti, M. Randeria, T.V. Ramakrishnan, and S.S. Mandal, Phys. Rev. B **62**, 6786 (2000).
[15] J.R. Schrieffer and A.P. Kampf, J. Phys. Chem. Solids **56**, 1673 (1995).
[16] P.A. Lee, N. Nagaosa, T.K. Ng, and X.-G. Wen, Phys. Rev. B **57**, 6003 (1998).
[17] P. W. Anderson, *The Theory of Superconductivity in the High-*T_c *Cuprate Superconductors* (Princeton University Press, Princeton, NJ, 1997).
[18] H. Fukuyama, Prog. Theor. Phys. Suppl. **108**, 287 (1992).
[19] D. Pines, Z. Phys. B: Condens. Matter **103**, 129 (1997).
[20] A. Paramekanti, M. Randeria, and N. Trivedi, Phys. Rev. Lett. **87**, 217002 (2001).
[21] I. Iguchi, T. Yamaguohl, and A. Suglmoto, Nature (London) **412**, 420 (2001).
[22] Z.A. Xu, N.P. Ong, Y. Wang, T. Kakeshita, and S. Uchida, Nature (London) **406**, 486 (2000).
[23] J.L. Tallon and J.W. Loram, Physica C **349**, 53 (2001).
[24] S. Chakravarty, R.B. Laughlin, Dirk K. Morr, and Chetan Nayak, Phys. Rev. B **63**, 094503 (2001); C. Nayak, *ibid.* **62**, 4880 (2000); **62**, R6135 (2000).
[25] M. Norman, H. Ding, M. Randeria, J.C. Campuzano, T. Yokoya, T. Takeuchi, T. Takahashi, T. Mochiku, K. Kadowaki, P. Guptasarma, and D.G. Hinks, Nature (London) **392**, 157 (1998).
[26] V.M. Krasnov, A. Yurgens, D. Winkler, P. Delsing, and T. Claeson, Phys. Rev. Lett. **84**, 5860 (2000).
[27] J.E. Sonier, J.H. Brewer, R.F. Kiefl, R.I. Miller, G.D. Morris, C.E. Stronach, J.S. Gardner, S.R. Dunsiger, D.A. Bonn, W.N. Hardy, R. Liang, and R.H. Heffner, Science **292**, 1692 (2001).
[28] J.-X. Zhu, W. Kim, C.S. Ting, and J.P. Carbotte, cond-mat/0105580 (unpublished); D.K. Morr, cond-mat/0106285 (unpublished); Q.-H. Wang, Phys. Rev. Lett. **88**, 057002 (2002); H.V. Kruis, I. Martin, and A.V. Balatsky, Phys. Rev. B **64**, 054501 (2001).
[29] Haranath Ghosh (unpublished).
[30] See also X.G. Wen and P.A. Lee, Phys. Rev. Lett. **76**, 503 (1996).
[31] E. M. Lifshitz and L. P. Pitaevskii, *Statistical Physics* (Pergamon, New York, 1991), Part II.
[32] Qiang-Hua Wang, Jung Hoon Han, and Dung-Hai Lee, Phys. Rev. Lett. **87**, 077004 (2001).
[33] M.R. Norman, M. Randeria, H. Ding, and J.C. Campuzano, Phys. Rev. B **52**, 615 (1995).
[34] H.A. Mook, D. Pai, S.M. Hayden, A. Hiens, J.W. Lynn, S.-H. Lee, and F. Dogam, cond-mat/0204002 (unpublished).