k-dependent SU(4) model of high-temperature superconductivity and its coherent-state solutions

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We extend the SU(4) model [Guidry *et al.*, Phys. Rev. B **63**, 134516 (2001); Wu *et al.*, Phys. Rev. B **67**, 014515 (2003); Guidry *et al.*, Phys. Rev. B **70**, 184501 (2004); Sun *et al.*, Phys. Rev. B **73**, 134519 (2006); Sun *et al.*, Phys. Rev. B **75**, 134511 (2007)] for high-T_c superconductivity to an $SU(4)_k$ model that permits explicit momentum (k) dependence in predicted observables. We derive and solve gap equations that depend on k, temperature, and doping from the $SU(4)_k$ coherent states, and we show that the present $SU(4)_k$ model reduces to the original SU(4) model for observables that do not depend explicitly on momentum. The results of the $SU(4)_k$ model are relevant for experiments such as angle-resolved photoemission spectroscopy (ARPES) that detect explicitly k-dependent properties. The present $SU(4)_k$ model describes quantitatively the pseudogap temperature scale and may explain why the ARPES-measured T^* along the antinodal direction is larger than the other measurements that do not resolve momentum. It also provides an immediate microscopic explanation for Fermi arcs observed in the pseudogap region. In addition, the model leads to a prediction that even in the underdoped regime, there exist doping-dependent windows around nodal points in the k space, where antiferromagnetism may be completely suppressed for all doping fractions, permitting pure superconducting states to exist.

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I. INTRODUCTION

The mechanism that leads to high-temperature superconductivity (SC) in the cuprates remains an open question despite intense study for the past two decades. Although the field has been challenged by many high-quality data from different types of measurement, there is no uniformly accepted theoretical picture that can offer a unified and consistent description for these data. It is often believed that underlying physics can be understood in terms of individual particles interacting through appropriately chosen interactions. However, even with greatly simplified Hamiltonians, describing collective motion in these strongly correlated many-electron systems has had only limited success. This has led some authors[1] to conclude that the many-body correlations in cuprates are so strong that dynamics may no longer be described meaningfully in terms of electrons and must be described instead in terms of new effective building blocks that fractionalize spin and charge.

Simplicity is a kind of beauty in physics. Even if one could solve the problem with the help of large-scale numerical calculations, such a practice may not be interesting because physics can be completely buried in the numerous configurations used in the calculation. On the other hand, alternative approaches to many-body problems have been proposed. One is the method of fermion dynamical symmetries.[2] This approach is based on the fact that collective motions in strongly correlated many-body systems are often governed by only a few collective degrees of freedom, and a quantum system exhibiting dynamical symmetries usually contains two or more competing collective modes. Once these degrees of freedom are identified and properly incorporated into a model, the problem may be considerably simplified and, most importantly, the physics in such approaches may become transparent.

This is the philosophy where the SU(4) model of high-temperature superconductivity[3–7] is based on. For cuprate systems we have proposed that the most relevant collective degrees of freedom are d-wave SC and antiferromagnetism (AF), and that coherent pairs (not individual particles) formed from two electrons (or holes) centered on adjacent lattice sites are appropriate dynamical building blocks of the wave function. The choice of this space, which is small in size but rich in physics, corresponds to a physically motivated truncation of the huge Hilbert space corresponding to the original problem.

It has been found[3] that the spin-singlet (D) and the spin-triplet (π) pair operators, when supplemented with the particle-hole-like operators for staggered magnetization (Q), spin (S), and charge constitute a 16-element operator set that is closed under a $U(4) \supset U(1) \times SU(4)$ algebra if the d-wave form factor $g(\boldsymbol{k})$ in D and π pair operators is replaced by $\mathrm{sgn}[g(\boldsymbol{k})]$. The U(1) factor corresponds to a charge-density wave that is independent of the SU(4) subspace because of the direct product. This implies that in the minimal U(4) model charge-density waves do not influence the AF-SC competition in lowest order and our discussions have been focused in the SU(4) subspace with its coherent-state approximation.[3,4] It has been further discovered[5] that the SU(4) symmetry is a consequence of non-double-occupancy—the constraint that each lattice site cannot have more than one valence electron. This suggests a fundamental relationship between SU(4) symmetry and Mott-insulator normal states at half filling for cuprate superconductors.

Thus, the SU(4) model has ingredients of competing AF and SC modes, d-wave D and π pairs [entering as "preformed pairs" that are mixtures of the two kinds of paired states under the SU(4) constraint[6]] in wave functions, and non-double-occupancy imposed by the symmetry.[5] All of

these appear to be relevant for the physics of cuprate superconductors. For the data that do not resolve an explicit k dependence, the coherent-state solutions of the SU(4) model (with properly adjusted parameters for effective interaction strengths) can consistently describe SC gaps, pseudogaps (PGs), and the corresponding transition temperatures T_c and T^* in cuprates, as demonstrated in Ref. 7.

However, there are experimental indications for explicit k dependence that are observed by experiments such as angle-resolved photoemission spectroscopy (ARPES).[8,9] These data probe electrons near the Fermi surface having particular k directions. To describe k dependence in energy gaps, we must extend our original SU(4) model by displaying explicit k dependence in the gap equations and their corresponding solutions. This is the goal of the present paper.

This paper is organized as follows. In Sec. II, we outline the SU(4) background by pointing out the assumptions made when the original k-independent SU(4) model was constructed. Sections III and IV are, respectively, devoted to the presentation of the present k-dependent SU(4)$_k$ model and the k-dependent gap equations obtained using the generalized coherent-state method. We solve these gap equations in Sec. V and give analytical solutions for the superconducting gap and the pseudogap. Finally, we discuss some immediate consequences of the SU(4)$_k$ model in Sec. VI, and a short summary is given in Sec. VII.

II. DYNAMICAL SYMMETRIES AND THE ORIGINAL SU(4) MODEL

Interactions in dynamical symmetry theories are determined by symmetry groups.[3] A general SU(4) Hamiltonian with pairing and AF interactions can be written as[10]

$$H = H_0 - V_d - V_\pi - V_q, \tag{1}$$

where H_0 is the single-particle (sp) energy, and V_d, V_π, and V_q are the two-body spin-singlet pairing, spin-triplet pairing, and AF interactions, respectively,

$$H_0 = \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}}, \tag{2a}$$

$$V_d = \sum_{\boldsymbol{k},\boldsymbol{k}'} G^0_{\boldsymbol{k}\boldsymbol{k}'} D^\dagger(\boldsymbol{k}) D(\boldsymbol{k}'), \tag{2b}$$

$$V_\pi = \sum_{\boldsymbol{k},\boldsymbol{k}'} G^1_{\boldsymbol{k}\boldsymbol{k}'} \vec{\pi}^\dagger(\boldsymbol{k}) \cdot \vec{\pi}(\boldsymbol{k}'), \tag{2c}$$

$$V_q = \sum_{\boldsymbol{k},\boldsymbol{k}'} \chi^0_{\boldsymbol{k}\boldsymbol{k}'} \vec{Q}(\boldsymbol{k}) \cdot \vec{Q}(\boldsymbol{k}'). \tag{2d}$$

The operators appearing in Eq. (2) can be expressed as

$$D^\dagger(\boldsymbol{k}) = g(\boldsymbol{k}) c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow}, \tag{3a}$$

$$\pi^\dagger_{ij}(\boldsymbol{k}) = g(\boldsymbol{k}) c^\dagger_{\boldsymbol{k}+\boldsymbol{q},i} c^\dagger_{\boldsymbol{k},j}, \tag{3b}$$

$$Q_{ij}(\boldsymbol{k}) = c^\dagger_{\boldsymbol{k}+\boldsymbol{q},i} c_{\boldsymbol{k},j}, \tag{3c}$$

where $\pi^\dagger_{ij}(\boldsymbol{k})$ and $Q_{ij}(\boldsymbol{k})$ are, respectively, tensor forms of $\vec{\pi}^\dagger(\boldsymbol{k})$ and $\vec{Q}(\boldsymbol{k})$. In Eq. (3), $c^\dagger_{\boldsymbol{k},i}$ creates an electron of momentum $\boldsymbol{k}$ and spin projection i, $j=1$ or 2 ($\equiv\uparrow$ or $\downarrow$), and $\boldsymbol{q}=(\pi,\pi,\pi)$ is an AF ordering vector. The d-wave form factor,

$$g(\boldsymbol{k}) = g(k_x,k_y) = \cos k_x - \cos k_y, \tag{4}$$

appears in Eqs. (3a) and (3b) because of strong experimental evidence that in cuprates, the coherent pairs exhibit d-wave orbital symmetry.[11] Thus energy gaps generally are k dependent,

$$\Delta_d(\boldsymbol{k}) = \sum_{\boldsymbol{k}'} G^0_{\boldsymbol{k}\boldsymbol{k}'} \langle D^\dagger(\boldsymbol{k}) \rangle, \tag{5a}$$

$$\Delta_\pi(\boldsymbol{k}) = \sum_{\boldsymbol{k}'} G^1_{\boldsymbol{k}\boldsymbol{k}'} \langle \pi^\dagger_z(\boldsymbol{k}') \rangle, \tag{5b}$$

$$\Delta_q(\boldsymbol{k}) = \sum_{\boldsymbol{k}'} \chi^0_{\boldsymbol{k}\boldsymbol{k}'} \langle Q_z(\boldsymbol{k}') \rangle. \tag{5c}$$

The discussion to this point is general and no approximations have been made. In our original k-independent SU(4) model,[3–7] we have introduced approximations through the following assumptions:

$$g(\boldsymbol{k}) \approx \mathrm{sgn}[g(\boldsymbol{k})] \tag{6a}$$

$$\varepsilon_{\boldsymbol{k}} \approx \varepsilon \tag{6b}$$

$$G^i_{\boldsymbol{k}\boldsymbol{k}'} \approx G^i \quad (i=0,1), \quad \chi^0_{\boldsymbol{k}\boldsymbol{k}'} \approx \chi^0. \tag{6c}$$

Assumption (6a) removes the k dependence from form factors in the pair operators, and assumptions (6b) and (6c), respectively, replace the sp energy and interaction strengths with k-independent constants. These approximations thus lead to k-independent gaps

$$\Delta_d = G^0 \langle D^\dagger \rangle \quad \Delta_\pi = G^1 \langle \pi^\dagger_z \rangle \quad \Delta_q = \chi^0 \langle Q_z \rangle, \tag{7}$$

which are expressed in terms of the collective operators

$$D^\dagger = \sum_{\boldsymbol{k}} \mathrm{sgn}[g(\boldsymbol{k})] c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow},$$

$$\pi^\dagger_{ij} = \sum_{\boldsymbol{k}} \mathrm{sgn}[g(\boldsymbol{k})] c^\dagger_{\boldsymbol{k}+\boldsymbol{q},i} c^\dagger_{\boldsymbol{k},j},$$

$$Q_{ij} = \sum_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}+\boldsymbol{q},i} c_{\boldsymbol{k},j}. \tag{8}$$

The preceding equations constitute the basis for discussions in Refs. 3–7, and all our previous SU(4) results are obtained within this framework. As most cuprate data presumably represent weighted averages over contributions of different k components, the original SU(4) scheme works well. In Ref. 6, we derived and solved k-independent (but temperature and hole-doping dependent) SU(4) gap equations and used the results to construct generic gap and phase diagrams. We compared the results with some representative cuprate data in Ref. 7 and found that for data that do not resolve an explicit k dependence, the coherent-state solutions of the original SU(4) model can consistently describe SC gaps, pseudogaps, and the corresponding transition temperatures T_c and T^*.

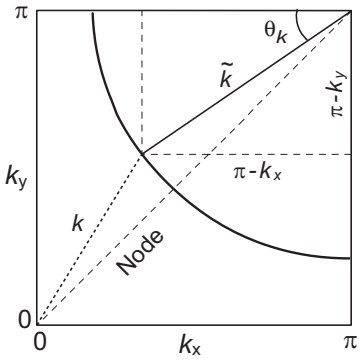

FIG. 1. Geometry and definitions in the k_x-k_y plane, where $\tilde{k}$ is hole momentum.

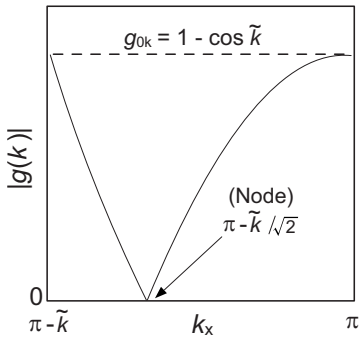

FIG. 2. The curve $|g(k)|$ and its maximum value $g_{0k}=1-\cos\tilde{k}$ for a given momentum $\boldsymbol{k}=(k_x,k_y)$ under constraint (11).

III. k-DEPENDENT SU(4)$_k$ MODEL

As we have noted, there is experimental evidence for explicit k dependence of certain observables in the cuprates. Although interpretation of some of the results remains somewhat controversial, their momentum-dependent nature is clear. One example is the observation of Fermi arcs in ARPES data:[8,9] ARPES measurements suggest that the Fermi surface is gapped out arcwise in the pseudogap region below T^*, indicating clear anisotropy of the PG in the k space.

In order to describe momentum dependence of energy gaps, we must extend our original SU(4) model[3–7] in a way that restores the k dependence that is washed out by the assumptions in Eq. (5) but preserves the SU(4) symmetry. The replacement (6a) for the pair operators is a necessary condition for preserving the SU(4) algebra,[3] which is required physically because it imposes the non-double-occupancy condition.[5] Therefore, the only way to restore k dependence in energy gaps but keep the SU(4) symmetry (and its associated non-double-occupancy constraint) is to modify Eqs. (6b) and (6c) to allow the sp energy ε and the interaction strengths to carry k dependence. The sp energy term ε is less important in this regard because it does not contribute to energy gaps and transition temperature in our formalism.[6] We may thus employ it in the most general form $\varepsilon_{\boldsymbol{k}}$.

Without loss of generality, $g(\boldsymbol{k})$ can be written as the product of the absolute value and a sign

$$g(\boldsymbol{k}) = |g(\boldsymbol{k})| \times \mathrm{sgn}[g(\boldsymbol{k})]. \tag{9}$$

Therefore, the approximation (6a) implies that in our original SU(4) model, we have assumed that the magnitude $|g(\boldsymbol{k})|$ is unity, regardless of $\boldsymbol{k}$. [Note that this is also the condition used to close the algebra of the SO(5) model.[12,13]] Instead of $|g(\boldsymbol{k})|=1$, we now introduce

$$|g(\boldsymbol{k})| \approx \sigma_{\boldsymbol{k}} = g_{0k}\delta(\theta_k), \tag{10}$$

where g_{0k} is the maximum value of $|g(\boldsymbol{k})|$. In Figs. 1 and 2, we illustrate the associated geometry and definitions. In our notation, $\boldsymbol{k}=(k_x,k_y)$ is the electron momentum under the constraint

$$(\pi - k_x)^2 + (\pi - k_y)^2 = \tilde{k}^2, \tag{11}$$

where $\tilde{k}$ is the hole momentum with θ_k as its azimuthal angle, as shown in Fig. 1. In Eq. (10), $\delta(\theta_k)$ takes a value of unity except in a narrow region around the nodal points (corresponding to $|k_x|=|k_y|$ or $\theta_k=\pm\pi/4$ for the first Brillouin zone; see Fig. 1), where it quickly diminishes and vanishes exactly at the nodal points. A possible mathematical expression could be of the Gaussian-type

$$\delta(\theta_k) = 1 - e^{-[(\theta_k - \pi/4)/\Delta\theta]^2} \quad \text{with} \quad \Delta\theta \ll \pi/4,$$

where $\Delta\theta$ measures the width of the Gaussian. With very small $\Delta\theta$, the exponential term has a negligible contribution to the average, which ensures that the averaged $\delta(\theta_k)$ is equal to 1. The so-defined $\delta(\theta_k)$ becomes exactly zero at $\theta_k=\pm\pi/4$. Therefore, our pairing gaps have nodes at $\theta_k=\pm\pi/4$, which agrees with experiments.

The behavior of $|g(\boldsymbol{k})|$ is illustrated in Fig. 2. It is easy to show that

$$g_{0k} = |1 - \cos\tilde{k}|. \tag{12}$$

Thus, for the first Brillouin zone k_x and k_y can take values from zero to π, while g_{0k} changes from 0 to 2. (The assumption $|g(\boldsymbol{k})|=1$ in the original SU(4) model is thus equivalent to taking an average of g_{0k} over $\boldsymbol{k}$.) Equation (10), with its explicit dependence on $\boldsymbol{k}$, clearly improves on the original SU(4) model for observables having a possible k dependence.

With approximation (10) for $|g(\boldsymbol{k})|$, the pairing interaction strengths in Eq. (2) are

$$G^i_{\boldsymbol{k}\boldsymbol{k}'} = G^0_i \sigma_{\boldsymbol{k}}\sigma_{\boldsymbol{k}'} \quad (i=0,1). \tag{13}$$

The factor $\mathrm{sgn}[g(\boldsymbol{k})]$ in the product (9) remains unchanged in the pair operators, which ensures preservation of the SU(4) symmetry.

The k dependence of the AF interaction $\chi_{\boldsymbol{k}\boldsymbol{k}'}$ follows from the nature of exchange interactions. The corresponding matrix elements are proportional to the wave-function overlap between the states, which are one-particle and one-hole states with momenta $(\boldsymbol{k}+\boldsymbol{q},\boldsymbol{k})$. The d-wave symmetry in the pair structure implies that the amplitude of a pair wave function with two electrons having momenta $(\boldsymbol{k},-\boldsymbol{k})$ in the background mean field of the SU(4) collective subspace is pro-

portional to $g(\boldsymbol{k})$. This means physically that the two electrons in a pair favor aligning their momenta $\boldsymbol{k}$ along the Cu-O bond direction [maximum of $|g(\boldsymbol{k})|$] rather than along the diagonal to the Cu-O bonds [nodal direction of $g(\boldsymbol{k})$; see Fig. 1]. Since the wave function for momentum $\boldsymbol{k}+\boldsymbol{q}$ differs from that for $\boldsymbol{k}$ only by a sign,[3] and a hole wave function is the conjugate of a particle wave function, the amplitude of a particle-hole wave function with momenta $(\boldsymbol{k}+\boldsymbol{q},\boldsymbol{k})$ should be very similar to that of a pair, and thus, proportional to $g(\boldsymbol{k})$. Therefore, we can write

$$\chi_{\boldsymbol{k}\boldsymbol{k}'} = \chi^0 g_{\boldsymbol{k}} g_{\boldsymbol{k}'}, \tag{14}$$

where $g_{\boldsymbol{k}} \equiv |g(\boldsymbol{k})|$. Note that for the $g_{\boldsymbol{k}}$ factor in Eq. (14), no approximation similar to the one in Eq. (10) is necessary. Explicitly, we mean here that $g_{\boldsymbol{k}}=|g(\boldsymbol{k})|=|\cos k_x - \cos k_y|$.

Inserting Eqs. (13) and (14) into Eq. (2), we can rewrite the Hamiltonian (1) as

$$H = \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}} - G_0^0 \sum_{\boldsymbol{k},\boldsymbol{k}'} \sigma_{\boldsymbol{k}}\sigma_{\boldsymbol{k}'} D^\dagger(\boldsymbol{k}) D(\boldsymbol{k}') - G_1^0 \sum_{\boldsymbol{k},\boldsymbol{k}'} \sigma_{\boldsymbol{k}}\sigma_{\boldsymbol{k}'} \vec{\pi}^\dagger(\boldsymbol{k}) \cdot \vec{\pi}(\boldsymbol{k}') - \chi^0 \sum_{\boldsymbol{k},\boldsymbol{k}'} g_{\boldsymbol{k}} g_{\boldsymbol{k}'} \vec{Q}(\boldsymbol{k}) \cdot \vec{Q}(\boldsymbol{k}'). \tag{15}$$

The k-dependent Hamiltonian (15) possesses a $\Sigma_k \otimes \mathrm{SU}(4)_k$ symmetry with 15 k-dependent generators

$$\mathbf{D}^\dagger(\boldsymbol{k}) = D^\dagger(\boldsymbol{k}) + D^\dagger(-\boldsymbol{k}),$$

$$\vec{\boldsymbol{\pi}}^\dagger(\boldsymbol{k}) = \vec{\pi}^\dagger(\boldsymbol{k}) + \vec{\pi}^\dagger(-\boldsymbol{k}),$$

$$\vec{\mathbf{Q}}(\boldsymbol{k}) = \vec{Q}(\boldsymbol{k}) + \vec{Q}(-\boldsymbol{k}),$$

$$\mathbf{M}(\boldsymbol{k}) = M(\boldsymbol{k}) + M(-\boldsymbol{k}),$$

$$\vec{\mathbf{S}}(\boldsymbol{k}) = \vec{S}(\boldsymbol{k}) + \vec{S}(-\boldsymbol{k}),$$

where $\mathbf{M}(\boldsymbol{k})$ and $\vec{\mathbf{S}}(\boldsymbol{k})$ are, respectively, the charge and the spin operators. For each $\boldsymbol{k}$, the commutation relation among generators, the structure of subgroup chains, and their corresponding properties are analogous to those of the original SU(4) group structure.[3] We term this k-dependent extension[14] of the original SU(4) model as the $\mathrm{SU}(4)_k$ model.

IV. k-DEPENDENT GAP EQUATIONS

In Sec. III, we demonstrated that with a better approximation to the absolute value of the form factor $g(\boldsymbol{k})$, it is possible to introduce explicit k dependence through a symmetry structure that corresponds to a product of SU(4) groups, each labeled by k. Therefore, the following discussions for gap equations and their solutions for a given k are rather similar to those in Ref. 6 for the k-independent SU(4) model.

By analogy with discussions in Appendix B of Ref. 6, under the coherent-state (symmetry-constrained generalized Hartree-Fock-Bogoliubov) approximation, one obtains for the k-dependent case

$$2u_{\boldsymbol{k}\pm} v_{\boldsymbol{k}\pm} (\varepsilon_{\boldsymbol{k}\pm} - \lambda) - \Delta_{\boldsymbol{k}\pm}(u_{\boldsymbol{k}\pm}^2 - v_{\boldsymbol{k}\pm}^2) = 0 \tag{16}$$

with

$$\varepsilon_{\boldsymbol{k}\pm} = \varepsilon_{\boldsymbol{k}} \mp \Delta_q(\boldsymbol{k}) \quad \Delta_{\boldsymbol{k}\pm} = \Delta_d(\boldsymbol{k}) \pm \Delta_\pi(\boldsymbol{k})$$

and

$$\Delta_d(\boldsymbol{k}) = G_0^0 \sigma_{\boldsymbol{k}} \sum_{\boldsymbol{k}'>0} \sigma_{\boldsymbol{k}'} \langle \mathbf{D}^\dagger(\boldsymbol{k}') \rangle,$$

$$\Delta_\pi(\boldsymbol{k}) = G_1^0 \sigma_{\boldsymbol{k}} \sum_{\boldsymbol{k}'>0} \sigma_{\boldsymbol{k}'} \langle \boldsymbol{\pi}_z^\dagger(\boldsymbol{k}') \rangle,$$

$$\Delta_q(\boldsymbol{k}) = \chi^0 g_{\boldsymbol{k}} \sum_{\boldsymbol{k}'>0} g_{\boldsymbol{k}'} \langle \mathbf{Q}_z(\boldsymbol{k}') \rangle.$$

$\boldsymbol{k}'>0$ in the above and following equations means $k_x'>0$ or $k_y'>0$. Solving Eq. (16) gives k-dependent occupation probabilities

$$u_{\boldsymbol{k}\pm}^2 = \frac{1}{2}\left[1 + \frac{\varepsilon_{\boldsymbol{k}\pm} - \lambda}{e_{\boldsymbol{k}\pm}}\right] \quad v_{\boldsymbol{k}\pm}^2 = \frac{1}{2}\left[1 - \frac{\varepsilon_{\boldsymbol{k}\pm} - \lambda}{e_{\boldsymbol{k}\pm}}\right]$$

and a quasiparticle energy

$$e_{\boldsymbol{k}\pm} = \sqrt{(\varepsilon_{\boldsymbol{k}\pm} - \lambda)^2 + \Delta_{\boldsymbol{k}\pm}^2}.$$

The gap equations in k space can then be obtained,

$$\Delta_d(\boldsymbol{k}) = \frac{G_0^0 \sigma_{\boldsymbol{k}}}{2} \sum_{\boldsymbol{k}'>0} \sigma_{\boldsymbol{k}'} (w_{\boldsymbol{k}'+}\Delta_{\boldsymbol{k}'+} + w_{\boldsymbol{k}'-}\Delta_{\boldsymbol{k}'-}), \tag{17a}$$

$$\Delta_\pi(\boldsymbol{k}) = \frac{G_1^0 \sigma_{\boldsymbol{k}}}{2} \sum_{\boldsymbol{k}'>0} \sigma_{\boldsymbol{k}'} (w_{\boldsymbol{k}'+}\Delta_{\boldsymbol{k}'+} - w_{\boldsymbol{k}'-}\Delta_{\boldsymbol{k}'-}), \tag{17b}$$

$$\Delta_q(\boldsymbol{k}) = \frac{\chi^0 g_{\boldsymbol{k}}}{2} \sum_{\boldsymbol{k}'>0} g_{\boldsymbol{k}'} \{ w_{\boldsymbol{k}'+}[\Delta_q(\boldsymbol{k}') + \lambda_{\boldsymbol{k}'}'] + w_{\boldsymbol{k}'-}[\Delta_q(\boldsymbol{k}') - \lambda_{\boldsymbol{k}'}'] \}, \tag{17c}$$

$$-2x = \frac{2}{\Omega} \sum_{\boldsymbol{k}'>0} \{ w_{\boldsymbol{k}'+}[\Delta_q(\boldsymbol{k}') + \lambda_{\boldsymbol{k}'}'] - w_{\boldsymbol{k}'-}[\Delta_q(\boldsymbol{k}') - \lambda_{\boldsymbol{k}'}'] \}, \tag{17d}$$

with

$$w_{\boldsymbol{k}\pm} = \frac{P_{\boldsymbol{k}\pm}(T)}{e_{\boldsymbol{k}\pm}} \quad \lambda_{\boldsymbol{k}}' = \lambda - \varepsilon_{\boldsymbol{k}},$$

$$P_{\boldsymbol{k}\pm}(T) = \tanh\left(\frac{e_{\boldsymbol{k}\pm}}{2k_B T}\right).$$

In Eq. (17d), $\Omega = \Sigma_{\boldsymbol{k}>0}$ is the maximum number of doped holes (or doped electrons for electron-doped compounds) that can form coherent pairs, assuming the normal state (at half filling) to be the vacuum. x is the relative doping fraction in the model.[6] Positive x represents the case of hole doping with $x=0$ corresponding to half filling (no doping)

and $x=1$ to maximal hole doping. The true doping P is related to x by $x \simeq 4P$.[6]

The k-dependent gap equations [Eq. (17)] are coupled algebraic equations. By solving these equations, one can in principle obtain k-dependent (also temperature and hole-doping dependent) energy gaps. However, general and exact solutions are difficult because gaps for given $\boldsymbol{k}$ are related to all other $\boldsymbol{k}$ points, which means that solutions at each $\boldsymbol{k}$ point are not independent from the other k components. In Sec. V, we show that one can obtain analytical solutions by applying some approximations.

V. SOLUTIONS FOR *k*-DEPENDENT GAP EQUATIONS

We may greatly simplify the solution of Eq. (17) through the following three steps. First, we replace the quantities in the summations on the right-hand side of Eq. (17) with their corresponding mean values,

$$\Delta_{\boldsymbol{k}\tau} \Rightarrow \bar{\Delta}_\tau(\tau = +,-,q) \quad \lambda'_{\boldsymbol{k}} \Rightarrow \bar{\lambda}',$$

$$w_{\boldsymbol{k}\pm} \Rightarrow \bar{w}_\pm \equiv \frac{\bar{P}_\pm(T)}{\bar{e}_\pm},$$

with

$$\bar{P}_\pm(T) = \tanh\left(\frac{\bar{e}_\pm}{2k_BT}\right) \quad \bar{e}_\pm = \sqrt{(\bar{\lambda}' \pm \bar{\Delta}_q)^2 + \bar{\Delta}_\pm^2}.$$

The functions $\sigma_{\boldsymbol{k}}$ and $g_{\boldsymbol{k}}$ in the summations can then be simplified as

$$\sum_{\boldsymbol{k}'>0} \sigma_{\boldsymbol{k}'} \Rightarrow \sum_{\boldsymbol{k}'>0} \bar{g}_0 = \frac{\Omega}{2}\bar{g}_0, \tag{18}$$

$$\sum_{\boldsymbol{k}'>0} g_{\boldsymbol{k}'} \Rightarrow \sum_{\boldsymbol{k}'>0} \bar{g} = \frac{\Omega}{2}\bar{g}. \tag{19}$$

The second level of simplification is based on physical considerations. Experimentally measured energy gaps are dominated by contributions from near the Fermi surface. Therefore, we assume that measured gaps may be approximated by their values at $\tilde{k}=k_f$. Using this approximation and the average values introduced in the first approximation step, we can write for the gap equations of Eq. (17) evaluated at $\tilde{k}=k_f$,

$$\Delta_d(\boldsymbol{k}) = \frac{\Omega}{4}G_0^0 g_0 \bar{g}_0 \delta(\theta_{k_f})(\bar{w}_+\bar{\Delta}_+ + \bar{w}_-\bar{\Delta}_-), \tag{20a}$$

$$\Delta_\pi(\boldsymbol{k}) = \frac{\Omega}{4}G_1^0 g_0 \bar{g}_0 \delta(\theta_{k_f})(\bar{w}_+\bar{\Delta}_+ - \bar{w}_-\bar{\Delta}_-), \tag{20b}$$

$$\Delta_q(\boldsymbol{k}) = \frac{\Omega}{4}\chi^0 g_0 \bar{g}\gamma(\theta_{k_f})\{\bar{w}_+[\bar{\Delta}_q + \bar{\lambda}'] + \bar{w}_-[\bar{\Delta}_q - \bar{\lambda}']\}, \tag{20c}$$

$$-2x = \bar{w}_+[\bar{\Delta}_q + \bar{\lambda}'] - \bar{w}_-[\bar{\Delta}_q - \bar{\lambda}'], \tag{20d}$$

where $g_0 \equiv g_{0k_f}$ and

$$\gamma(\theta_{k_f}) \equiv \left|\frac{g(\boldsymbol{k})}{g_0}\right|. \tag{21}$$

Equation (20) are k-dependent gap equations constrained on the Fermi surface through

$$(\pi - k_x)^2 + (\pi - k_y)^2 = k_f^2. \tag{22}$$

It can be shown that $\gamma(\theta_{k_f})$ is independent of $|k_f|$ to high accuracy, and therefore, can be considered in later discussions to be a function of azimuthal angle only.

In the third simplification step, we assume the average values $\bar{\Delta}_\tau$ and $\bar{\lambda}'$ to be proportional to the unknown quantities $\Delta_\tau(\boldsymbol{k})$ and $\lambda'_{\boldsymbol{k}}$, respectively, with a constant of proportionality R,

$$\bar{\Delta}_\tau = R\Delta_\tau(\boldsymbol{k}) \quad (\tau = +,-,q), \quad \bar{\lambda}' = R\lambda'_{\boldsymbol{k}}, \tag{23}$$

which implies that

$$\bar{e}_\pm = Re_{\boldsymbol{k}\pm}. \tag{24}$$

The parameter R serves as a renormalization factor that corrects on average the errors caused by the approximation and is determined by the fitting data. With Eq. (23), Eq. (20) now becomes

$$\Delta_d(\boldsymbol{k}) = \frac{\Omega}{4}G_0\delta(\theta_{k_f})[\tilde{w}_+\Delta_+(\boldsymbol{k}) + \tilde{w}_-\Delta_-(\boldsymbol{k})], \tag{25a}$$

$$\Delta_\pi(\boldsymbol{k}) = \frac{\Omega}{4}G_1\delta(\theta_{k_f})[\tilde{w}_+\Delta_+(\boldsymbol{k}) - \tilde{w}_-\Delta_-(\boldsymbol{k})], \tag{25b}$$

$$\Delta_q(\boldsymbol{k}) = \frac{\Omega}{4}\chi\frac{\gamma(\theta_{k_f})}{\bar{\gamma}}\{\tilde{w}_+[\Delta_q(\boldsymbol{k}) + \lambda'_{\boldsymbol{k}}] + \tilde{w}_-[\Delta_q(\boldsymbol{k}) - \lambda'_{\boldsymbol{k}}]\}, \tag{25c}$$

$$-2x = \tilde{w}_+[\Delta_q(\boldsymbol{k}) + \lambda'_{\boldsymbol{k}}] - \tilde{w}_-[\Delta_q(\boldsymbol{k}) - \lambda'_{\boldsymbol{k}}], \tag{25d}$$

with

$$G_i = G_i^0 g_0 \bar{g}_0, \quad \chi = \chi^0 g_0 \bar{\gamma}\bar{g}$$

and

$$\tilde{w}_\pm = \frac{\tilde{P}_\pm(T)}{e_{\boldsymbol{k}\pm}} \quad \tilde{P}_\pm(T) = \tanh\left(\frac{Re_{\boldsymbol{k}\pm}}{2k_BT}\right). \tag{26}$$

In the above equations, $\bar{\gamma}$ is the average value of $\gamma(\theta_{k_f})$.

The simplified gap Eq. (25) can now be solved analytically. They have the same structure as the gap equations discussed in the k-independent SU(4) model,[6] except that the interaction strengths in the present case are k anisotropic. Therefore, all the SU(4) formulas in Secs. III–VI of Ref. 6 remain valid, provided that the following replacements are made for the singlet-pairing, triplet-pairing, and antiferromagnetic coupling strengths, respectively,

$$G_0 \to G_0\delta(\theta_{k_f}), \quad G_1 \to G_1\delta(\theta_{k_f}), \quad \chi \to \chi\gamma(\theta_{k_f})/\bar{\gamma}. \tag{27}$$

For example, if we introduce the doping parameter x defined in Sec. IIC of Ref. 6, the k-dependent critical hole-doping fraction is [compare Eq. (23) of Ref. 6]

$$x_{q\theta} \equiv x_q(\theta_{k_f}) = \sqrt{\frac{\chi\gamma(\theta_{k_f})/\bar{\gamma} - G_0\delta(\theta_{k_f})}{\chi\gamma(\theta_{k_f})/\bar{\gamma} - G_1\delta(\theta_{k_f})}}, \tag{28}$$

and the $T=0$ energy gaps at the Fermi momentum k_f for $x \leq x_{q\theta}$ are obtained as

$$\Delta_d(\boldsymbol{k}) = \frac{\Omega}{2}G_0\delta(\theta_{k_f})\sqrt{x(x_{q\theta}^{-1} - x)}, \tag{29a}$$

$$\Delta_\pi(\boldsymbol{k}) = \frac{\Omega}{2}G_1\delta(\theta_{k_f})\sqrt{x(x_{q\theta} - x)}, \tag{29b}$$

$$\Delta_q(\boldsymbol{k}) = \frac{\Omega}{2}\chi\frac{\gamma(\theta_{k_f})}{\bar{\gamma}}\sqrt{(x_{q\theta}^{-1} - x)(x_{q\theta} - x)}, \tag{29c}$$

$$\lambda_{\boldsymbol{k}}' = -\frac{\Omega}{2}\left[\chi\frac{\gamma(\theta_{k_f})}{\bar{\gamma}} - G_1\delta(\theta_{k_f})\right]x_{q\theta}(1 - x_{q\theta}x) - \frac{\Omega}{2}G_1\delta(\theta_{k_f})x, \tag{29d}$$

while for $x > x_{q\theta}$ we obtain $\Delta_q(\boldsymbol{k}) = \Delta_\pi(\boldsymbol{k}) = 0$ and

$$\Delta_d(\boldsymbol{k}) = \frac{\Omega}{2}G_0\delta(\theta_{k_f})\sqrt{1 - x^2} \tag{30a}$$

$$\lambda_{\boldsymbol{k}}' = -\frac{\Omega}{2}G_0\delta(\theta_{k_f})x \tag{30b}$$

for the solutions. The energy gaps obtained in Eqs. (29) and (30) are k anisotropic. The pairing gaps have nodal points at $k_x = k_y$, where $\delta(\theta_{k_f}) = 0$. The pseudogap $\Delta_q(\boldsymbol{k})$ is a function of $\boldsymbol{k}$ by virtue of the factor $\gamma(\theta_{k_f})$ defined in Eq. (21).

Because all SU(4) formulas in Secs. III–VI of Ref. 6 remain valid, it is easily proven that the PG closure temperature T^* acquires the same $g(\boldsymbol{k})$ dependence as the pseudogap, and we obtain for the PG closure temperature

$$T^*(\boldsymbol{k}) = \chi\frac{\gamma(\theta_{k_f})}{\bar{\gamma}}\Omega\frac{R(1 - x^2)}{4k_B}. \tag{31}$$

We do not expect a corresponding effect in the superconducting region because below T_c, the pairing gap opens and the entire Fermi surface will be destroyed except at the nodal points. We find a superconducting transition temperature

$$T_c(\boldsymbol{k}) = G_0\delta(\theta_{k_f})\Omega\frac{Rx}{4k_B\,\mathrm{arctanh}(x)}, \tag{32}$$

which has no $g(\boldsymbol{k})$ factor.

VI. DISCUSSIONS AND PREDICTIONS

Most experimental techniques do not resolve k and we expect for those that transition temperatures are dominated by contributions from near the Fermi surface ($\tilde{k} = k_f$), which are averaged over all k directions. If one takes the average over θ_{k_f}, then

$$\delta(\theta_{k_f}) \to 1, \quad \gamma(\theta_{k_f})/\bar{\gamma} \to 1,$$

and the gap equations of the k-dependent $SU(4)_k$ model and their solutions become identical to those obtained for the original k-independent SU(4) model.[6] Thus our original SU(4) model predicts[6,7] values of energy gaps and the corresponding transition temperatures that are (perhaps weighted) *averages over k*. These are relevant for comparison with experiments that do not resolve k. However, the explicit appearance of the anisotropic factor $\gamma(\theta_{k_f})/\bar{\gamma}$ in the gap solutions of the $SU(4)_k$ model leads to some interesting consequences. We note that although our following discussions are made through the anisotropic factor $\gamma(\theta_{k_f})/\bar{\gamma}$, its relation with $\delta(\theta_{k_f})$ guarantees that the model still preserves the d-wave nature and has nodes in the pairing gaps. In this section we discuss three predictions following from the present formalism that could have important implications for experiments that detect explicitly k-dependent properties.

A. Two pseudogap closure temperatures: The maximum and the averaged

The k-dependent PG closure temperature $T^*(\boldsymbol{k})$ in Eq. (31) differs from the k-averaged one derived in Eq. (49) of Ref. 6,

$$T_{\mathrm{av}}^* = \chi\Omega\frac{R(1 - x^2)}{4k_B}, \tag{33}$$

by the factor $\gamma(\theta_{k_f})/\bar{\gamma}$. We know that $\gamma(\theta_{k_f})$ and also $T^*(\boldsymbol{k})$ take their maximum values at the antinodal points, for example,

$$\gamma_{\max}(\theta_{k_f})|_{\theta_{k_f}=0,\pi/2} = 1$$

(see Figs. 1 and 2). We can denote the maximum PG closure temperature as $T_{\max}^*$. Thus, the $SU(4)_k$ model predicts two PG closure temperatures that are related to each other through

$$T_{\max}^* = T_{\mathrm{av}}^*/\bar{\gamma}. \tag{34}$$

It is straightforward to evaluate the averaged γ value by integration. Noting that Eqs. (29a)–(29d) are restricted to $x \leq x_{q\theta}$, we can define the maximum allowed azimuthal angle θ_c through the condition $x = x_{q\theta}(\theta_c)$. We then have

$$\bar{\gamma} = \frac{2}{\pi}\int_0^{\theta_c}\left|\frac{g[k(\theta)]}{g_0}\right|d\theta. \tag{35}$$

In the above calculation, we have used for the integrand expression (21) for $\gamma(\theta_{k_f})$ and constraint (22). The resulting $\bar{\gamma}$ depends on the size of the Fermi surface $|k_f|$. Assuming an isotropic hole Fermi surface, we have

$$k_f^2 = 2\pi(1 + P).$$

Therefore, $\bar{\gamma}$ is essentially a hole-doping-dependent quantity. In Fig. 3, we show the behavior of $1/\bar{\gamma}$ as a function of

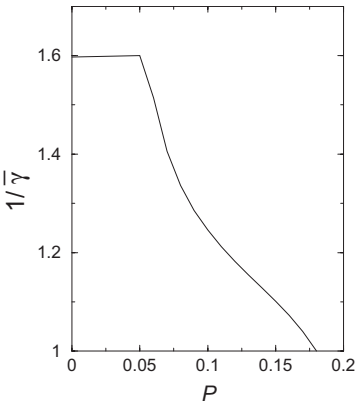

FIG. 3. The doping-dependent $1/\bar{\gamma}$ factor. The calculation employs Eq. (35) and utilizes realistic interaction strengths χ, G_0, and G_1 taken from Ref. 7 with the pairing onset at $P=0.05$.

doping P, assuming coupling-strength parameters that are characteristic of the cuprate superconductors. As one can see, it has a nonlinear dependence on doping, taking the maximum value of 1.6 at very small dopings, falling rapidly between $P=0.05$ and 0.08, and decreasing continuously but with a smaller rate until it reaches unity at the critical doping $P=0.18$.

We thus obtain two distinct PG closure temperatures, $T^*_{\rm av}$ and $T^*_{\rm max}$, having the same microscopic origin[6,7] but differing in the kinds of experimental observables for which they are appropriate. The largest difference between the two is found for small doping; they take similar values at large dopings, becoming identical at the optimal doping point. In Ref. 7, experimental values of T_c and T^* (Ref. 15) that do not resolve k were compared to our theoretical T_c and $T^*_{\rm av}$. In Fig. 4, we replot these values in green for T_c (with open triangles for data and dotted curve for theory) and blue for $T^*_{\rm av}$ (with open squares for data and solid curve for theory). Above the blue (solid) curve, we now add the maximum PG closure temperatures $T^*_{\rm max}$ in red (with open circles for data and dashed curve for theory). Because of the $1/\bar{\gamma}$ factor shown in Fig. 3, the red (dashed) curve lies well above the blue (solid) curve at low dopings. In Ref. 16, Campuzano *et al.* reported their ARPES data (plotted as red circles in Fig. 4). In the underdoped regime it is clear that the results from Refs. 15 and 16 differ substantially. Because the ARPES experiment typically detects k-dependent properties, we suggest that the data from Ref. 16 actually measure $T^*_{\rm max}$, as predicted in the present paper, while the data cited in Ref. 15 measure the k-averaged $T^*_{\rm av}$, as described in our earlier paper.[7] We emphasize that in this interpretation the two types of experiments are seeing the *same underlying physics*, but the observations differ because what is actually being measured differs in the two cases.

B. Temperature-dependent Fermi arcs

The pseudogap closure temperature $T^*(\boldsymbol{k})$ is anisotropic in $\boldsymbol{k}$. Combining Eqs. (31), (33), and (34), we have

$$T^*(\boldsymbol{k}) = T^*_{\rm max}\gamma(\theta_{k_f}) = \frac{T^*_{\rm max}}{g_0}|g(k_f)|, \tag{36}$$

where the doping-dependent quantity $T^*_{\rm max}$ is the maximum value of $T^*(\boldsymbol{k})$ in the antinodal direction, $\theta_{k_f}=0$ or $\pi/2$. For

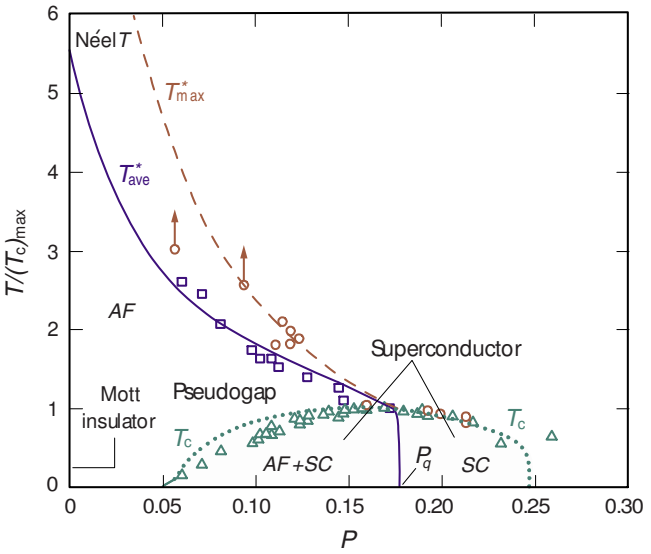

FIG. 4. (Color online) SU(4) cuprate phase diagram compared with data. Strengths of the AF and singlet-pairing correlations were determined in Ref. 7 by global fits to cuprate data. The PG temperature is T^* and the SC transition temperature is T_c. The AF correlations vanish, leaving a pure singlet d-wave condensate above the critical doping P_q. Dominant correlations in each region are indicted by italic labels. Data in green (open triangles) and blue (open squares) are taken from Ref. 15 and those in red (open circles) are from Ref. 16 (arrows indicate that the point is a lower limit).

an arbitrary temperature $T<T^*_{\rm max}$, the k-dependent pseudogap closes when $T=T^*(\boldsymbol{k})$, which is equivalent to the requirement that

$$|\cos k_x - \cos k_y| = g_0(T/T^*_{\rm max}) \tag{37}$$

upon substituting Eqs. (4) and (36). This equation says that the magnitude of the d-wave form factor (4) that expresses the nodal structure[11] in cuprate superconductors is proportional to the scaled quantity $T/T^*_{\rm max}$ with a proportionality factor g_0 that is related to the size of the Fermi surface.

Simultaneous solution of Eqs. (22) and (37) gives values of k_x and k_y where the pseudogap closes at a given P and T. Figure 5 illustrates the solution of Eqs. (22) and (37) graphically for several temperatures at fixed doping. The solution of Eq. (37) is represented by the curves bounding the shaded regions, and the solution of Eq. (22) is represented by the Fermi-surface curves in each corner. The intersection of these curves defines two simultaneous solutions in each of the four quadrants that bound the surviving part of the Fermi surface (heavier portions of the curves in Fig. 5). In the shaded portions of Fig. 5 the Fermi surface has been destroyed by the pseudogap, leaving only a vestigial Fermi arc between the shaded regions.

The solution in Fig. 5 represents a derivation of Fermi-arc structure expected in the underdoped regime above T_c. Below T_c, the Fermi surface is completely destroyed by the opening of the pairing gap except at the nodal point since the pairing gap has no $\gamma(\theta_{k_f})$ dependence [see Eq. (29)]. We emphasize that the calculations presented in Fig. 5 do not

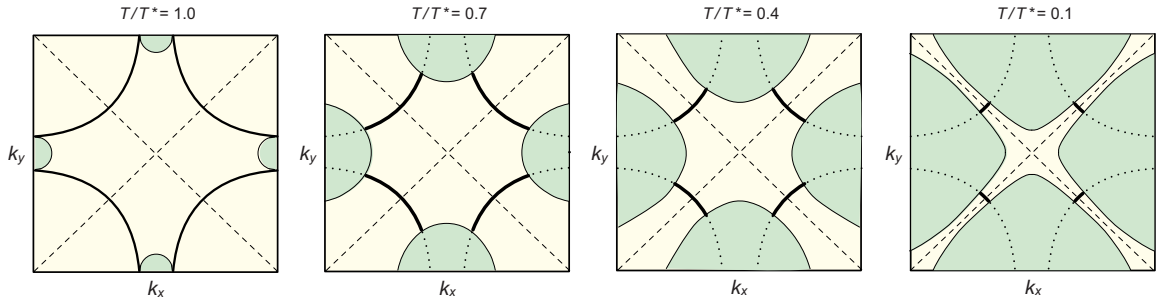

FIG. 5. (Color online) Construction of Fermi arcs for doping $P=0.15$ and values of $T/T^*_{\max}$ decreasing left to right. The ranges of k_x and k_y are from $-\pi$ to π and dashed lines indicate nodes. Hole Fermi surfaces in the absence of gaps are illustrated by full solid arcs in each corner. For $T \geq T^*_{\max}$ a full Fermi surface exists; for $T < T^*_{\max}$, opening of the pseudogap destroys Fermi surfaces in the shaded regions (dotted lines), leaving arcs (solid lines) centered on the nodal lines. These arcs have absolute lengths that depend on P and T but relative lengths that depend only very weakly on P and are determined almost entirely by the ratio $T/T^*_{\max}$. The sizes of the shaded regions grow with decreasing T, so at very low temperature almost all of the Fermi surface becomes gapped and the Fermi arcs shrink to the nodal points as $T/T^*_{\max} \rightarrow 0$.

involve any additional parameters as long as the PG closure temperatures have been calculated (presented in Fig. 4).

Kanigel *et al.*[9] reported from their ARPES experiment arclengths for slightly underdoped Bi2212. A direct reading of the Fermi arclength from Fig. 5 permits us to compare it quantitatively with the Kanigel data. Details will be published elsewhere.[17]

C. Complete suppression of antiferromagnetism: Pure superconducting states in underdoped compounds

As we have discussed extensively in Ref. 6, the antiferromagnetic correlation that plays a key role in understanding underdoped cuprates is completely suppressed at and beyond the critical doping point x_q. A pure (d wave) BCS superconducting state occurs at zero temperature in the overdoped portion of the phase diagram. We now show that a similar situation can also occur in certain k windows in the *underdoped* regime, in which AF correlation is completely suppressed and a pure SC state emerges.

This is another interesting consequence of the $SU(4)_k$ model due to the anisotropic factor $\gamma(\theta_{k_f})/\bar{\gamma}$. The critical doping point defined in Eq. (28), which is constant in the k-averaged SU(4) model,[6] is now a function of momentum direction θ_{k_f} because of the anisotropic factor $\gamma(\theta_{k_f})/\bar{\gamma}$. Consequently, for each given doping x there always exists a window in the momentum azimuthal angle, $\theta_c < \theta_{k_f} < (\pi/2 - \theta_c)$, and centering at the nodal point $\pi/4$ within which the AF correlation vanishes and only the pairing gap Δ_d exists. This follows because inside the window $x_{q\theta} < x$; therefore, solution (29) is not permitted but solution (30) is. The critical angle θ_c is determined by the condition $x_{q\theta}(\theta_c) = x$. Figure 6 illustrates the situation.

Because $\gamma(\theta_{k_f})/\bar{\gamma}$, and thus $x_{q\theta}$, is a doping-dependent quantity, the above phenomenon depends on doping. The sequential figures, plotted for four different dopings in Fig. 7, show the behavior of the energy gaps as functions of the momentum direction. Whenever

$$x = x_q = \sqrt{\frac{\chi - G_0}{\chi - G_1}},$$

$\theta_c = 0$, which means that there is no momentum space available to Δ_q and Δ_π, and the AF correlations and triplet-pairing states are completely suppressed. Therefore, for $x \geq x_q$ the system can only be in a pure superconducting state at zero temperature. It can be seen that larger doping x implies a smaller critical angle θ_c, and thus, a wider pairing window, and that the width of the pairing window decreases rapidly toward zero as the doping goes to zero.

In the original SU(4) model, we found that the critical doping point defines a natural boundary (quantum phase transition) between underdoped and overdoped regimes that have qualitatively different wave functions.[6] We termed the underdoped superconducting regime the AF+SC phase (antiferromagnetic superconducting phase); it is characterized by having all gaps nonzero but is dominated by AF and SC gaps. The present extension to the $SU(4)_k$ model reveals the additional feature that in this AF+SC phase, the gaps are *highly anisotropic* in the momentum space, implying the possibility of a pure SC window around the nodal points even in the underdoped regime. The proposed existence of these pure superconducting windows may have considerable implication for the nature of the Fermi surface at low doping, for the Nernst effect, and for the relationship of impurities to inhomogeneities in the underdoped region. These deserve further investigation.

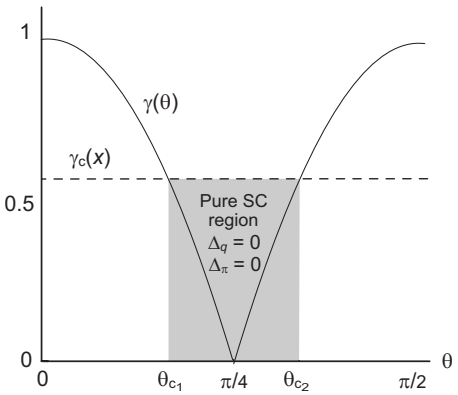

FIG. 6. The anisotropic factor $\gamma(\theta)$. In this figure, $\theta_{c1} = \theta_c$, $\theta_{c2} = \pi/2 - \theta_c$, and θ_c is determined by $x_{q\theta}(\theta_c) = x$. The value of $\gamma(\theta)$ at the critical angle θ_c is denoted by $\gamma(\theta_c) \equiv \gamma_c(x)$, where $\gamma_c(x)$ is a monotonically increasing function of doping x that becomes equal to unity when $x = x_q$.

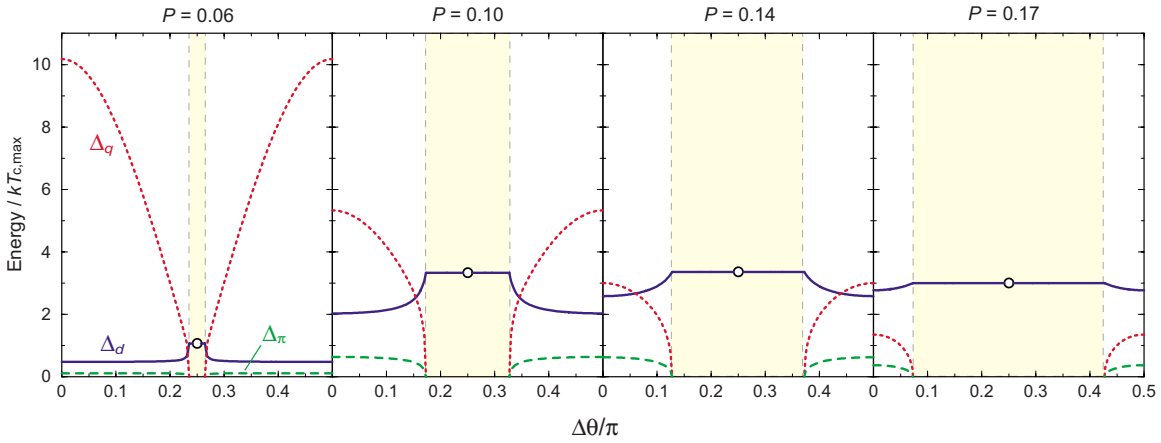

FIG. 7. (Color online) Dependence of the energy gaps Δ_d, Δ_π, and Δ_q on the momentum direction θ for several representative dopings P. For each doping there is a θ window (yellow shaded region) centered at the node $\theta=\pi/4$ (indicated by the open circle), in which $\Delta_q=\Delta_\pi=0$, and $\Delta_d\neq 0$. This window encompasses only a few percent of the Brillouin zone at low doping (tending to zero at zero doping) but rapidly expands to fill the entire Brillouin zone near the critical doping $P\simeq 0.18$ and beyond.

The above analysis has assumed $T=0$ for simplicity, but the basic picture should be valid also in the case with nonzero temperature. The formulation and solution of the gap equations described in this paper can be extended to finite temperature using the methods described in Ref. 7. While of considerable practical importance, this extension does not involve conceptually different ideas and will be deferred to a later paper.

VII. SUMMARY

In this paper, we have extended the SU(4) model for high-T_c superconductivity to include explicit momentum dependence in observables. To do so, we have started from a general SU(4) Hamiltonian and introduced a better approximation for the *d*-wave form factor in the pair operators. This leads to the present $SU(4)_k$ model, which retains explicit k dependence while preserving SU(4) symmetry. We have solved the gap equations derived from the $SU(4)_k$ coherent states with some plausible approximations, obtaining analytical solutions for k-dependent superconducting gaps, pseudogaps, and their transition temperatures T_c and T^*. The present $SU(4)_k$ model reduces to the original SU(4) model for observables that are averaged over all possible k directions. Therefore we propose that the original SU(4) model describes the averaged features and thermal properties of cuprates, while the present $SU(4)_k$ model presented in this paper extends this description to detailed anisotropic properties in the k space. The present results have been obtained for zero temperature but the formalism presented here may be extended to finite temperature in a manner similar to the extension of the k-averaged SU(4) model.

Because of an anisotropic factor $\gamma(\theta_{k_f})/\bar{\gamma}$ in the analytical gap solutions, the cuprate phase structure in the underdoped regime becomes even richer than that for k-averaged observations. We have discussed three immediate consequences that emerge in the present $SU(4)_k$ model.

(1) We have suggested the possibility of two distinct and measurable pseudogap closure temperatures: the maximum and the averaged. In the coherent-state SU(4) theory the pseudogap could be interpreted either as arising from competing AF and SC degrees of freedom, or alternatively as fluctuations of pairing subject to SU(4) constraints.[6,7] The proposed $T^*_{\rm av}$ and $T^*_{\rm max}$ share the same microscopic origin but differ from each other by a doping-dependent factor. The temperature $T^*_{\rm av}$ represents PG closure temperatures that are averages over k, while $T^*_{\rm max}$, which is generally higher than $T^*_{\rm av}$, represents the pseudogap temperature expected if one retains explicit k dependence. Experimentally, then, we predict that $T^*_{\rm av}$ is the pseudogap temperature that should be measured in experiments that do not resolve k explicitly, but (the generally higher) $T^*_{\rm max}$ is the expected measured pseudogap temperature for experiments such as ARPES that resolve k.

(2) We have provided a theoretical framework to understand ARPES Fermi-arc data. Using two analytical equations, we have obtained a solution for the T/T^*-dependent Fermi arclengths that is in quantitative agreement with existing measurements. The essence of this result is the appearance of the factor $\gamma(\theta)$ in the PG closure temperature that has been derived in Eq. (31).

(3) We have predicted the existence of doping-dependent windows in the momentum space where antiferromagnetic correlation is completely suppressed in the underdoped regime. Without AF competition, it is possible for pure superconducting states to emerge in these windows. Thus, we find that pure BCS-type superconducting states can exist not only in conventional superconductors or in overdoped cuprate high-T_c superconductors (where such behavior is well established) but also in localized islands even in underdoped cuprate superconductors. It is of interest whether this prediction is related to the recent observation of small pockets of well-defined Fermi surface in underdoped cuprate superconductors.

Some of these predictions (for example, the two temperature scales for pseudogap behavior) have the potential to reconcile apparent discrepancies in existing data. All make predictions that can be tested in experiments capable of resolving k-dependent behavior.

Finally, we note that the recent discovery of superconductivity in layered iron-based transition-metal oxypnictides[18] has generated a new wave of research interest. In place of copper and oxygen, the new compounds contain iron and arsenic, and the highest critical temperature for them has already reached 55 K.[19] It has been demonstrated in neutron-scattering experiments[20] that, similar to high-T_c copper oxides, superconductivity in these iron-based materials is likely competing strongly with antiferromagnetic degrees of freedom. It will be of considerable interest to see whether approaches similar to the one presented in this paper, or other models capable of handling multiple competing degrees of freedom in strongly correlated systems on an equal footing, can explain these new high-temperature superconductors and their relationship to the old ones.[21] In particular, we note that what is already known about the iron-based superconductors suggests that k-dependent phenomena of the sort described in this paper should also be observable in these new superconductors.

[1] P. W. Anderson, Physica C **341-348**, 9 (2000); D. Pines, *ibid.* **341-348**, 59 (2000); B. Laughlin and D. Pines, Proc. Natl. Acad. Sci. U.S.A. **97**, 28 (2000).

[2] C.-L. Wu, D. H. Feng, and M. W. Guidry, Adv. Nucl. Phys. **21**, 227 (1994).

[3] M. W. Guidry, L.-A. Wu, Y. Sun, and C.-L. Wu, Phys. Rev. B **63**, 134516 (2001).

[4] L.-A. Wu, M. W. Guidry, Y. Sun, and C.-L. Wu, Phys. Rev. B **67**, 014515 (2003).

[5] M. W. Guidry, Y. Sun, and C.-L. Wu, Phys. Rev. B **70**, 184501 (2004).

[6] Y. Sun, M. W. Guidry, and C.-L. Wu, Phys. Rev. B **73**, 134519 (2006).

[7] Y. Sun, M. W. Guidry, and C.-L. Wu, Phys. Rev. B **75**, 134511 (2007).

[8] M. R. 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).

[9] A. Kanigel, M. R. Norman, M. Randeria, U. Chatterjee, S. Souma, A. Kaminski, H. M. Fretwell, S. Rosenkranz, M. Shi, T. Sato, T. Takahashi, Z. Z. Li, H. Rarry, K. Kadowaki, D. Hinks, L. Ozyuzer, and J. C. Campuzano, Nat. Phys. **2**, 447 (2006).

[10] We assume that total spin is conserved and is zero for the ground state. Charge-density wave and spin-wave degrees of freedom are ignored at the minimal level.

[11] D. J. Scalapino, Phys. Rep. **250**, 329 (1995).

[12] S. Rabello, H. Kohno, E. Demler, and S.-C. Zhang, Phys. Rev. Lett. **80**, 3586 (1998).

[13] C. L. Henley, Phys. Rev. Lett. **80**, 3590 (1998).

[14] Extension of the SU(4) algebra to the k-dependent case has also been worked out independently by J. Dukelsky, B. Errea, S. Lerma, and J. Dukelsky (private communication).

[15] P. Dai, H. A. Mook, S. M. Hayden, G. Aeppli, T. G. Perring, R. D. Hunt, and F. Dogan, Science **284**, 1344 (1999); M. Oda, K. Hoya, R. Kubota, C. Manabe, N. Momono, T. Nakano, and M. Ido, Physica C **281**, 135 (1997); T. Watanabe, T. Fujii, and A. Matsuda, Phys. Rev. Lett. **84**, 5848 (2000); B. Wuyts, V. V. Moshchalkov, and Y. Bruynseraede, Phys. Rev. B **53**, 9418 (1996); M. Takigawa, A. P. Reyes, P. C. Hammel, J. D. Thompson, R. H. Heffner, Z. Fisk, and K. C. Ott, *ibid.* **43**, 247 (1991); T. Ito, K. Takenaka, and S. Uchida, Phys. Rev. Lett. **70**, 3995 (1993).

[16] J. C. Campuzano, H. Ding, M. R. Norman, H. M. Fretwell, M. Randeria, A. Kaminski, J. Mesot, T. Takeuchi, T. Sato, T. Yokoya, T. Takahashi, T. Mochiku, K. Kadowaki, P. Guptasarma, D. G. Hinks, Z. Konstantinovic, Z. Z. Li, and H. Raffy, Phys. Rev. Lett. **83**, 3709 (1999).

[17] M. W. Guidry, Y. Sun, and C.-L. Wu, arXiv:0705.0822 (unpublished).

[18] Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, J. Am. Chem. Soc. **130**, 3296 (2008).

[19] Z.-A. Ren, W. Lu, J. Yang, W. Yi, X.-L. Shen, C. Zheng, G.-C. Che, X.-L. Dong, L.-L. Sun, F. Zhou, and Z.-X. Zhao, Chin. Phys. Lett. **25**, 2215 (2008).

[20] C. de la Cruz, Q. Huang, J. W. Lynn, J. Li, W. Ratcliff II, J. L. Zarestky, H. A. Mook, G. F. Chen, J. L. Luo, N. L. Wang, and P. Dai, Nature (London) **453**, 899 (2008).

[21] Y. Sun, M. Guidry, and C.-L. Wu, Chin. Sci. Bull. **53**, 1617 (2008).