Intralayer and interlayer spin-singlet pairing and energy gap functions with different possible symmetries in high-T_c layered superconductors

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Anisotropy and the wave-vector dependence of the energy gap function determine many important properties of a superconductor. Starting from first principles, we present here a complete analysis of possible symmetries of the superconducting gap function $E_g(\mathbf{k})$ at the Fermi surface in high-T_c layered superconductors with either a simple orthorhombic or a tetragonal unit cell. This is done within the framework of Gorkov's mean-field theory of superconductivity in the so-called ''layer representation'' introduced by us earlier. For N conducting cuprate layers, $J=1,2,\ldots,N$, in each unit cell, the spin-singlet order parameters $\Delta_{JJ'}(\mathbf{k})$ can be expanded in terms of possible basis functions of all the irreducible representations relevant to layered crystals, which are obtained here. In layered materials, the symmetry is restricted to the translational lattice periodicity in the direction perpendicular to the layers and the residual point group and translational symmetries for the two-dimensional unit cell in each layer of the three-dimensional unit cell. We derive an exact general relation to determine different branches of the energy gap function $E_g(\mathbf{k})$ at the Fermi surface in terms of $\Delta_{JJ'}(\mathbf{k})$, which include both intralayer and interlayer order parameters. For $N=2$, we also obtain an exact expression for quasiparticle energies $E_p(\mathbf{k})$, $p=1,2$, in the superconducting state in the presence of intralayer and complex interlayer order parameters as well as complex tunneling matrix elements between the two layers in the unit cell, which need not be equivalent. The form of the possible basis functions are also listed in terms of cylindrical coordinates k_t,ϕ,k_z to take advantage of the orthogonality of functions with respect to ϕ integrations. In layered materials, with open Fermi surfaces in the k_z direction, there is orthogonality of basis functions with respect to k_z also $(-\pi \leqslant k_z d \leqslant \pi)$. Our results show that in orthorhombic systems, planar $d_{k_x^2-k_y^2}$-like (B_{1g}) and $d_{k_xk_y}$-like (B_{2g}) symmetries are always mixed, respectively, with the planar s-wave-like (A_{1g}) and A_{2g}-like symmetries of the corresponding tetragonal system. There is also the possibility of a weak modulation of $E_g(\mathbf{k})$ as a function of $k_z(\sim\cos k_z d)$. In addition, in the presence of interlayer pairings which may or may not have the same symmetry as the intralayer order parameters, even in tetragonal systems the nodes of the $d_{k_x^2-k_y^2}$-like intralayer gap function will be shifted. In view of this, some suggestions for analyzing experimental data are also presented. [S0163-1829(97)02922-6]

I. INTRODUCTION

The problem of the actual symmetry and the wave-vector dependence of the spin-singlet pairing gap function $\Delta(\mathbf{k})$ in high-T_c cuprate superconductors has attracted great attention[1,2] during the last several years, because of its unconventional behavior in comparison to its almost isotropic form in low-T_c materials. Since the anisotropy and the $\mathbf{k}$ dependence of the energy gap function, including its possible nodes at the Fermi surface, determine the nature of quasiparticle excitations and various important properties of a superconductor, the significance of knowing its form for practical applications of these materials cannot be minimized. This is also important from the theoretical point of view if we have to move towards a proper understanding of the superconducting pairing in these materials at a more basic level. Although recent Josephson coupling experiments,[1] along with several other types of observations, have shown evidence[3] for a planar $d_{k_x^2-k_y^2}$-like symmetry in some high-T_c materials, which seems to be consistent with the usual Berk-Schrieffer form for the spin-fluctuation exchange mechanism[4,5] in CuO_2 layers in the Hubbard model, there are many other experiments[2] which give either anisotropic extended s-wave-like or mixed s-wave and d-wave-like symmetries, as far as the dependence of the gap function on $\mathbf{k}_t=(k_x,k_y)$ in the layer plane is concerned. In reality, there need not be any universal behavior in all high-T_c cuprates, but the answer is still not clear.

High-T_c cuprate superconductors are known to be layered materials, with orthorhombic or tetragonal unit-cell symmetry, and very weak interaction and single-particle tunneling between the layers. It is assumed that holes or electrons in CuO_2 layers of each unit cell are directly involved in the spin-singlet pairing in these materials.[6] Other layers in the unit cell contribute to the superconducting state of these materials only indirectly through their weak coupling to CuO_2 layers. In such a layered system, it is, therefore, more appropriate to characterize the superconducting state in terms of possible intralayer pairing order parameters $\Delta_{JJ}(\mathbf{k}_t,k_z)$ and interlayer pairing order parameters $\Delta_{JJ'}(\mathbf{k}_t,k_z)$, $J\neq J'$,

where J and J' label the CuO_2 layers in a unit cell, and where $\mathbf{k}_t$ and k_z are the wave vector in the layer plane and in the direction perpendicular to it. Instead of the usual expression for the energy gap at the Fermi surface, $2\Delta(\mathbf{k})$, in the familiar one-band three-dimensional case, where $\Delta(\mathbf{k})$ is the corresponding energy gap function, the energy gap is now determined by the set of order parameters $\Delta_{JJ'}(\mathbf{k}_t,k_z)$; $J,J'=1,2,\ldots,N$, where N is the number of superconducting layers per unit cell. In order to tackle this problem effectively, we have already developed[7] a microscopic framework for spin-singlet pairing theory of superconductivity in such layered materials, in terms of a general effective dynamical interaction, $V(\mathbf{r}_1,\mathbf{r}_2,\omega)$, between the charge carriers, and an appropriate set of single-particle electronic states defining the so-called ''layer'' representation. To start with, for simplicity, this theory was applied to the case of N-equivalent layers per unit cell, with only intralayer pairing independent of $\mathbf{k}_t$ (i.e., isotropic s-wave-like in the layer plane), to study the saturation[7,8] properties of the superconducting transition temperature T_c as a function of N, and the anisotropy[7,9] of the gap parameters $\Delta_{JJ}(k_z)$ as a function of k_z. The case of two layers per unit cell, with both intralayer and interlayer pairings, were also considered in great detail[7] in terms of phenomenological pairing interactions, but the analysis was again restricted to the case of $\mathbf{k}_t$-independent order parameters. For two equivalent layers per unit cell, the energy gap function for the resulting two branches was given by $E_g=\Delta(k_z)\pm\Delta_\perp(k_z)$, where $\Delta=\Delta_{11}=\Delta_{22}$ was the real intralayer pairing order parameter, and $\Delta_\perp(k_z)=|\Delta_{12}(k_z)|=|\Delta_{21}(-k_z)|$ was the amplitude of the interlayer pairing order parameter. Note that in our notation, the minimum energy gap for pair breaking is $2E_g$.

In view of the possibility of unconventional symmetry and $\mathbf{k}_t$ dependence of the intralayer order parameters in the layer plane, recently we used our approach to analyze[10] this situation for layered systems with either orthorhombic or tetragonal symmetry in the case of N-equivalent layers per unit cell, with no interlayer pairings. We showed that for tetragonal systems there is a possibility of pure planar d-wave-like symmetry for the order parameters $\Delta_{JJ}(\mathbf{k}_t,k_z)$ near $T=T_c$, apart from its weak modulation ($\sim\cos k_z d$, where d is the length of the unit cell in the z direction) as a function of k_z. In orthorhombic systems, planar $d_{k_x^2-k_y^2}$-like symmetry is always mixed with the planar s-wave-like symmetry. Since interlayer pairing is expected to mix planar symmetries even in the tetragonal case, it is important to extend our analysis to the most general case where both intra- and interlayer pairings are considered simultaneously, with various possible basis functions which are consistent with the symmetry of the conducting layers in the unit cell of the crystal. To be more particular and focused, in this paper we will address this general problem in greater detail for the case of two layers ($N=2$) per unit cell. Based on this, we will then discuss the case of arbitrary number of layers per unit cell. Our work is expected to establish a sound basis to analyze past and future experimental data exploring the possible symmetry of the superconducting state in high-T_c layered crystals.

In Sec. II of this paper, we will briefly review our earlier formulation[7] of the generalized pairing theory of superconductivity in layered materials within the framework of the Gorkov mean-field theory. This will establish the notation for our layer representation and the corresponding mathematical framework. The formulation is in terms of the normal-state single-particle Green function $g(\mathbf{r}_1,\mathbf{r}_2,\omega)$ and the general effective dynamical interaction $V(\mathbf{r}_1,\mathbf{r}_2,\omega)$, both in our layer representation. It includes the possibility of both intralayer and interlayer pairings. A general expression for the energy gap function $E_g(\mathbf{k})$ for quasiparticle excitations at the Fermi surface in terms of the order parameters $\Delta_{JJ'}(\mathbf{k})$, $J,J'=1,2,\ldots,N$, is also derived in this section. For layered crystals, with orthorhombic or tetragonal symmetry, it is enough to consider the periodicity of the unit cell in the z direction, perpendicular to the layers, and the corresponding residual two-dimensional point-group and translational symmetry for each CuO_2 layer in the unit cell. To be complete and to avoid confusion, in Sec. III we obtain and list the possible irreducible representations (IRR's) and their basis functions which can be used to expand order parameters $\Delta_{JJ'}(\mathbf{k})$ and $E_g(\mathbf{k})$, in simple tetragonal and orthorhombic layered systems. Basis functions are also given in terms of the cylindrical coordinates k_t,ϕ,k_z, since in layered crystals with widely open Fermi surfaces, the integrations over $k_z d$ and ϕ cover the full period in each case, so that the orthogonality of the basis functions in these coordinates can be used in our analysis.

The problems of one layer ($N=1$) and two layers ($N=2$) per unit cell are examined in detail in Sec. IV, with various possible symmetries for the order parameters and the energy gap function $E_g(\mathbf{k})$. For two layers per unit cell, which need not be equivalent, we also give an exact expression for the two branches of the quasiparticle energy $E(\mathbf{k})$, in the presence of intralayer and interlayer pairings as well as complex tunneling matrix elements between the layers. In Sec. V, we briefly consider the general case of N layers per unit cell. In particular, we emphasize how one can analyze the symmetry of the energy gap function $E_g(\mathbf{k})$ in this case, if the interlayer pairings are allowed only between the nearest-neighbor layers in the unit cell. We conclude our paper in Sec. VI with a short discussion.

II. MATHEMATICAL FRAMEWORK FOR THE SPIN-SINGLET PAIRING THEORY IN A LAYERED CRYSTAL

For describing the generalized pairing theory in layered materials, it is convenient to introduce the Bloch-periodic layer representation[7] for the single-particle electronic states in terms of a set of orthonormalized functions $\chi_{na\mathbf{k}_t\sigma}(x,y,z-z_{nM})$ localized at different layers in the crystal. Here, the vertical z coordinate of the nth layer in the Mth vertical unit cell has been denoted by $z_{nM}=z_n+Md$, where d is the unit-cell length in the z direction perpendicular to the layers, and σ refers to the effective spin-up and spin-down states which are degenerate in the absence of any external magnetic field. The functions $\chi_{na\mathbf{k}_t\sigma}(\mathbf{r})$ are products of two-dimensional Bloch-like band functions, labeled by the band index ''a'' and the layer wave vector $\mathbf{k}_t=(k_x,k_y)$ in the $x-y$ layer plane, and one-dimensional Wannier-like functions in the z direction localized at different layers in the crystal. They

satisfy the orthonormalization conditions

$$\int d^3r \chi^*_{n'a'\mathbf{k}'_t\sigma}(x,y,z-z_{n'M'})\chi_{na\mathbf{k}_t\sigma}(x,y,z-z_{nM}) = \delta_{n'n}\delta_{M'M}\delta_{a'a}\delta_{\mathbf{k}'_t,\mathbf{k}_t}. \quad (1)$$

The basis functions for each of the layers n in any unit cell of the crystal, which define our Bloch-periodic layer representation are then just the Bloch sum

$$L_{na\mathbf{k}\sigma}(\mathbf{r}) = \langle \mathbf{r}|na\mathbf{k}\sigma\rangle = \frac{1}{\sqrt{N_3}}\sum_M e^{ik_zMd}\chi_{na\mathbf{k}_t\sigma}(x,y,z-z_n-Md); \quad -\pi/d \leqslant k_z \leqslant \pi/d, \quad (2)$$

where N_3 is the number of unit cells in the vertical z direction of the crystal. Note that the above basis functions are not the eigenstates of the three-dimensional Bloch Hamiltonian H_0, and there are still nonvanishing single-particle ''tunneling'' matrix elements of H_0 between different layers in the unit cell. Since the extension of the single-particle energy bandwidth in the k_z direction is expected to be very narrow and small compared to the Fermi energy μ in any highly layered metal, all states with $-\pi/d \leqslant k_z \leqslant \pi/d$ are occupied at the Fermi surface (FS). In other words, the Fermi surface is expected to be widely open in the direction perpendicular to the reciprocal layer $\mathbf{k}_t$ plane.

In the Gorkov decoupling scheme, the generalized pairing theory of superconductivity is described[7] in terms of the single-particle Green functions $G^{\sigma\sigma'}(x_1,x_2) = -\langle T(\psi_\sigma(x_1)\psi^\dagger_{\sigma'}(x_2))\rangle$; $\overline{G}^{\sigma\sigma'}(x_1,x_2) = -\langle T(\psi^\dagger_\sigma(x_1)\psi_{\sigma'}(x_2))\rangle = -G^{\sigma'\sigma}(x_2,x_1)$, and the anomalous Green functions $F^{\sigma\sigma'}(x_1x_2) = -\langle P^\dagger T(\psi_\sigma(x_1)\psi_{\sigma'}(x_2))\rangle$, $\overline{F}^{\sigma\sigma'}(x_1,x_2) = -\langle PT(\psi^\dagger_\sigma(x_1)\psi^\dagger_{\sigma'}(x_2))\rangle$, where x stands for $(\mathbf{r},it)$, T is the usual time-ordering operator, and P and $P^\dagger$ change $(N+2)$ and $(N-2)$-particle states to the N-particle state. The self-energies corresponding to the anomalous Green functions $F^{\sigma\sigma'}$ and $\overline{F}^{\sigma\sigma'}$, in the presence of the effective dynamic pairing interaction $V(\mathbf{r}_1,\mathbf{r}_2,i\omega_m - i\omega_{m'})$, where the Matsubara frequencies $\omega_m = (2m+1)\pi k_BT$, $m = 0,\pm1,\pm2,\ldots$, are the gap functions $\Delta^{\sigma\sigma'}$ and $\overline{\Delta}^{\sigma\sigma'}$, with

$$\Delta^{\sigma\sigma'}(\mathbf{r}_1,\mathbf{r}_2,i\omega_m) = k_BT\sum_{m'} V(\mathbf{r}_1,\mathbf{r}_2,i\omega_m - i\omega_{m'}) \times F^{\sigma\sigma'}(\mathbf{r}_1,\mathbf{r}_2,i\omega_{m'}), \text{ etc.} \quad (3)$$

In the absence of pairing in the normal state, the single-particle Green functions $G^{\sigma\sigma'}$ and $\overline{G}^{\sigma\sigma'}$ are supposed to be given by $g^{\sigma\sigma'}$ and $\overline{g}^{\sigma\sigma'}$. Then the full set of self-consistent generalized Gorkov equations for superconductivity, with the possibility of both spin-singlet and spin-triplet pairings, are given by

$$G^{\sigma_1\sigma_2}(\mathbf{r}_1,\mathbf{r}_2,i\omega_m) = g^{\sigma_1\sigma_2}(\mathbf{r}_1,\mathbf{r}_2,i\omega_m) + \int d^3r_3\int d^3r_4 \times \sum_{\sigma_3}\sum_{\sigma_4} g^{\sigma_1\sigma_3}(\mathbf{r}_1,\mathbf{r}_3,i\omega_m)\Delta^{\sigma_3\sigma_4} \times (\mathbf{r}_3,\mathbf{r}_4,i\omega_m)\overline{F}^{\sigma_4\sigma_2}(\mathbf{r}_4,\mathbf{r}_2,i\omega_m), \quad (4)$$

$$\overline{F}^{\sigma_1\sigma_2}(\mathbf{r}_1,\mathbf{r}_2,i\omega_m) = \int d^3r_3\int d^3r_4 \times \sum_{\sigma_3}\sum_{\sigma_4} \overline{g}^{\sigma_1\sigma_3}(\mathbf{r}_1,\mathbf{r}_3,i\omega_m)\overline{\Delta}^{\sigma_3\sigma_4} \times (\mathbf{r}_3,\mathbf{r}_4,i\omega_m)G^{\sigma_4,\sigma_2}(\mathbf{r}_4,\mathbf{r}_2,i\omega_m) \quad (5)$$

with similar equations for $\overline{G}^{\sigma_1\sigma_2}$ and $F^{\sigma_1\sigma_2}$, where in Eqs. (4) and (5), $g \leftrightarrow \overline{g}$, $\Delta \leftrightarrow \overline{\Delta}$, $G \leftrightarrow \overline{G}$, and $F \leftrightarrow \overline{F}$.

If we restrict ourselves only to the spin-singlet pairing, in the absence of any external magnetic field, the generalized pairing theory can be written down in terms of the single-particle Green function $G = G^{\uparrow\uparrow} = G^{\downarrow\downarrow}$, the singlet anomalous Green function F_s and the corresponding gap function Δ_s, together with the two input functions, namely, the normal-state Green function $g = g^{\uparrow\uparrow} = g^{\downarrow\downarrow}$ and the effective pairing interaction function V. They are represented by Eqs. (1)–(3) in the first paper of Ref. 7 (to be referred to as I, hereafter). For the sake of clarity, if we further restrict this exposition to an effective Hamiltonian in which only the conducting layers, $J = 1,2,\ldots,N$, in each unit cell, are directly involved in the pairing, with only one two-dimensional band for each layer, one can rewrite the set of these three equations of the spin-singlet theory in terms of a set of three equations for $N\times N$ matrices $\underline{G}$, $\underline{F}$, and $\underline{\Delta}$ in the layer representation. Using the following expansions and notations:

$$G(\mathbf{r}_1,\mathbf{r}_2,i\omega_m) = \sum_{\mathbf{k}}\sum_{J_1,J_2} L_{J_1\mathbf{k}\sigma}(\mathbf{r}_1)L^*_{J_2\mathbf{k}\sigma}(\mathbf{r}_2)G_{J_1J_2}(k), \quad (6)$$

$$F_s(\mathbf{r}_1,\mathbf{r}_2,i\omega_m) = \sum_{\mathbf{k}}\sum_{J_1,J_2} L^*_{J_1,-\mathbf{k}\downarrow}(\mathbf{r}_1)L^*_{J_2,\mathbf{k}\uparrow}(\mathbf{r}_2)F_{J_1J_2}(k) = \sum_{\mathbf{k}}\sum_{J_1,J_2} L_{J_1\mathbf{k}\uparrow}(\mathbf{r}_1)L_{J_2,-\mathbf{k}\downarrow}(\mathbf{r}_2)F_{J_1J_2}(k), \quad (7)$$

$$\Delta_s(\mathbf{r}_1,\mathbf{r}_2,i\omega_m) = \sum_{\mathbf{k}}\sum_{J_1,J_2} L_{J_1\mathbf{k}\uparrow}(\mathbf{r}_1)L_{J_2,-\mathbf{k}\downarrow}(\mathbf{r}_2)\Delta_{J_1J_2}(k) = \sum_{\mathbf{k}}\sum_{J_1,J_2} L^*_{J_1,-\mathbf{k}\downarrow}(\mathbf{r}_1)L^*_{J_2,\mathbf{k}\uparrow}(\mathbf{r}_2)\Delta_{J_1J_2}(k), \quad (8)$$

$$g(\mathbf{r}_1,\mathbf{r}_2,i\omega_m) = \sum_{\mathbf{k}}\sum_{J_1,J_2} L_{J_1\mathbf{k}\sigma}(\mathbf{r}_1)L^*_{J_2\mathbf{k}\sigma}(\mathbf{r}_2)g_{J_1J_2}(k) \quad (9)$$

$$V_{J_1J_2;J_3J_4}(k,k')=V_{J_1J_2;J_3J_4}(\mathbf{k},\mathbf{k}',i\omega_m-i\omega_{m'})$$
$$=\langle J_1\mathbf{k}\uparrow;J_2,-k\downarrow|V(\mathbf{r}_1,\mathbf{r}_2,i\omega_m-i\omega_{m'})$$
$$\times|J_3\mathbf{k}'\uparrow,J_4,-\mathbf{k}'\downarrow\rangle, \tag{10}$$

$$k\equiv(\mathbf{k},i\omega_m)=(\mathbf{k}_t,k_z,i\omega_m);$$

$$k'\equiv(\mathbf{k}',i\omega_{m'})=(\mathbf{k}_t',k_z',i\omega_{m'}) \tag{11}$$

the resulting set of self-consistent coupled $N\times N$ matrix equations for the spin-singlet pairing theory for layered metals are given by

$$\underline{G}(k)=\underline{g}(k)+\underline{g}(k)\underline{\Delta}(k)\underline{F}(k), \tag{12}$$

$$\underline{F}(k)=-\underline{g}^{\text{trans}}(-k)\underline{\Delta}(k)\underline{G}(k) \tag{13}$$

$$[\underline{\Delta}(k)]_{J_1J_2}=\sum_{k'}\sum_{J_3,J_4}V_{J_1J_2;J_3J_4}(k,k')F_{J_3J_4}(k')$$
$$\equiv\left[\sum_{k'}\underline{V}(k,k')F(k')\right]_{J_1J_2}, \tag{14}$$

where the matrix $\underline{g}^{\text{trans}}$ is the usual transpose of the matrix $\underline{g}$, related to $\underline{g}^t$ of I by

$$g^{\text{trans}}_{J_1J_2}(-k)=g_{J_2J_1}(-k)=g^t_{J_1J_2}(k). \tag{15}$$

In the above set of Eqs. (12)–(14), the super matrix $\underline{V}$ is defined in Eq. (14) itself, and the summation over k' implies,

$$\sum_{k'}\cdots\equiv k_BT\sum_{\omega_{m'}}\int\frac{d^2k_t'}{(2\pi)^2}\int_{-\pi/d}^{\pi/d}\frac{dk_z'}{(2\pi/d)}\cdots \tag{16}$$

for an open Fermi surface in the k_z direction.

The set of coupled Eqs. (12)–(14) has the formal solutions for $\underline{G}$ and $\underline{\Delta}$ which can be rewritten in the form

$$\underline{G}(k)=\underline{g}(k)[\underline{I}+\underline{\Delta}(k)\underline{g}^{\text{trans}}(-k)\underline{\Delta}(k)\underline{g}(k)]^{-1}, \tag{17}$$

$$\underline{\Delta}(k)=-\sum_{k'}\underline{V}(k,k')[[\underline{g}^{\text{trans}}(-k')\underline{\Delta}(k')\underline{g}(k')]$$
$$\times[\underline{I}+\underline{\Delta}(k')\underline{g}^{\text{trans}}(-k')\underline{\Delta}(k')\underline{g}(k')]^{-1}], \tag{18}$$

where $\underline{I}$ is the unit $N\times N$ matrix, and the inverse of any matrix has the usual definition.

Note that near $T\sim T_c$, when $\underline{\Delta}$ is small, one has the linearized form of Eq. (18), whose nontrivial solution corresponding to the maximum possible T_c determines the superconducting state. One has to solve the linear eigenvalue equation

$$\underline{\Delta}(k)=-\sum_{k'}\underline{V}(k,k')[\underline{g}^{\text{trans}}(-k')\underline{\Delta}(k')\underline{g}(k')],\quad T=T_c, \tag{19}$$

in which the summation over k' includes the summation over $\omega_{m'}=(2m'+1)\pi k_BT_c$, $m'=0,\pm1,\pm2,\ldots$.

In general, when we analytically continue $\Delta(i\omega_m)$ to real frequencies ω, the gap function $\Delta(\mathbf{k},\omega)$ is a complex function, even for a single layer per unit cell. However, because of its analytic properties in the ω plane, it satisfies the usual Kramer's-Krönig relations between its real and imaginary parts, with $\Delta(\omega)=\Delta^*(-\omega)$. If the frequencies involved in the pairing exchange mechanism are large compared to k_BT_c, one may assume that Δ is almost frequency independent up to the frequencies of the order of a few times k_BT_c, with a negligible imaginary part in that low-frequency region. For the spin-singlet pairing, because of the requirement of symmetric spatial part, one has also the relation [examine, e.g., Eq. (8)]

$$\Delta_{J_1J_2}(\mathbf{k})=\Delta_{J_2J_1}(-\mathbf{k}). \tag{20}$$

Similarly, the pairing interaction $V_{JJ,JJ}(\mathbf{k},\mathbf{k}',i\omega_m-i\omega_{m'})$ is symmetric with respect to the interchange of $\mathbf{k}$ and $\mathbf{k}'$, etc., and the transformation $\mathbf{k}\rightarrow-\mathbf{k}$, $\mathbf{k}'\rightarrow-\mathbf{k}'$.

The poles of the normal-state Green function in the ω plane in the representation in which it is diagonal, $\underline{S}^{-1}\underline{g}\underline{S}\equiv\underline{g}^{(\alpha)}$ (diagonal), represent the normal-state single-particle energies and their damping. If one ignores the imaginary part and the frequency dependence of the normal-state self-energy, one can assume a simplified form

$$g^{(\alpha)}_{\alpha\alpha'}(\mathbf{k},i\omega_m)=(i\omega_m-\xi_\alpha)^{-1}\delta_{\alpha\alpha'},\quad \alpha=1,2,\ldots,N \tag{21}$$

for it in the α representation in which it is diagonal. Exactly at the Fermi surface, defined by $\xi_\alpha=0$ for all the N sheets ($\alpha=1,2,\ldots,N$), $\underline{g}^{(\alpha)}$ reduces to the form $(i\omega_m)^{-1}\underline{I}$. In other words, exactly at the Fermi surface (FS), in the layer representation also, $\underline{g}=\underline{S}\underline{g}^{(\alpha)}\underline{S}^{-1}=(i\omega_m)^{-1}\underline{I}$, and one has

$$\underline{g}^{-1}(\mathbf{k},i\omega_m)=i\omega_m\underline{I},$$
$$\underline{g}^{\text{trans}}(-\mathbf{k},-i\omega_m)=-(i\omega_m)^{-1}\underline{I},\quad\text{at FS}. \tag{22}$$

We also know that the poles of the full Green function $\underline{G}(\mathbf{k},\omega)$ in the ω plane, or the zeroes of the determinant of $\underline{G}^{-1}(\mathbf{k},\omega)$ determine the quasiparticle excitation energies E_p in the superconducting state. Exactly at the Fermi surface, with all $\xi_\alpha=0$, they can be identified with the energy gap functions E_{gp} for the N branches. In fact, Eqs. (17) and (22) imply that these poles are determined by the vanishing of the determinant

$$\det|\underline{\Delta}\underline{\Delta}-E_g^2\underline{I}|=0,\quad i\omega_m\rightarrow E_g \tag{23}$$

in the layer representation. This can be rewritten, after factorization, in the simpler form

$$\det|\underline{\Delta}\mp E_g\underline{I}|=0. \tag{24}$$

In other words, if $\underline{\Delta}$ can be assumed to be frequency independent, the eigenvalues of $\underline{\Delta}(\mathbf{k})$, with the appropriate choice of their sign, give the energy gap functions E_{gp}, $p=1,2,\ldots,N$. In particular, for $N=2$, (two layers per unit cell), with

$$\underline{\Delta}(\mathbf{k})=\begin{pmatrix}\Delta_{11}(\mathbf{k}) & \Delta_{12}(\mathbf{k})\\ \Delta_{21}(\mathbf{k}) & \Delta_{22}(\mathbf{k})\end{pmatrix} \tag{25}$$

in the J-J' layer representation, the two branches of the energy gap function are given by

$$(\pm)E_{g1,2}=\tfrac{1}{2}\,[\Delta_{11}(\mathbf{k})+\Delta_{22}(\mathbf{k})]\pm\tfrac{1}{2}\,[(\Delta_{11}(\mathbf{k})-\Delta_{22}(\mathbf{k}))^2 + 4\Delta_{12}(\mathbf{k})\Delta_{21}(\mathbf{k})]^{1/2}, \tag{26}$$

where one may assume, $\Delta_{JJ}(\mathbf{k})=\Delta_{JJ}(-\mathbf{k})$ to be real, and $\Delta_{21}(\mathbf{k})=\Delta_{12}(-\mathbf{k})=\Delta_{12}^{*}(\mathbf{k})$. Note that the $(\pm)$ sign in the left-hand side of the above equation represents the choice of any overall sign for E_g.

III. LAYER-SYMMETRY AND BASIS FUNCTIONS FOR ORDER PARAMETERS AND ENERGY-GAP FUNCTIONS $E_g(\mathbf{k})$

In general, the symmetry of $\underline{\Delta}(\mathbf{k})$ as a function of the three-dimensional wave vector $\mathbf{k}$ is determined by the translational and point-group symmetry of the unit cell of the crystal. Because of the lattice periodicity, it satisfies the relation

$$\underline{\Delta}(\mathbf{k}+\mathbf{G})=\underline{\Delta}(\mathbf{k}), \tag{27}$$

where $\mathbf{G}$ is any reciprocal-lattice vector. For the spin-singlet pairing, one in addition has the relation (20): $\Delta_{J_1J_2}(\mathbf{k})=\Delta_{J_2J_1}(-\mathbf{k})$. Similarly, the interaction function $\underline{V}(\mathbf{k},\mathbf{k}')$ is invariant under the transformation $\mathbf{k}\rightarrow\mathbf{k}+\mathbf{G}$ and $\mathbf{k}'=\mathbf{k}'+\mathbf{G}$. Any such function $f(\mathbf{k})$, satisfying the condition (27), can of course be expanded in terms of the direct lattice vectors $\mathbf{R}$,

$$f(\mathbf{k})=\sum_{\{\mathbf{R}\}} f(\mathbf{R})e^{i\mathbf{k}\cdot\mathbf{R}}=\sum_{\Gamma} f_\Gamma\psi_\Gamma(\mathbf{k}), \tag{28}$$

in which one can rearrange the plane waves $e^{i\mathbf{k}\cdot\mathbf{R}}$ in terms of the basis functions $\psi_\Gamma(\mathbf{k})$ for each irreducible representation (IRR) Γ of the point group. Since high-T_c cuprates occur as orthorhombic or tetragonal crystals with highly layered unit cells, it is better for us to consider only the residual symmetries and the corresponding basis functions for expanding the order parameters and pairing interactions, which are relevant to layered systems. We will assume that the layered crystal has the translational lattice symmetry in the z direction perpendicular to the layers, and the residual two-dimensional (2D) translational and point-group symmetry for the planar unit cell in each layer. For example, for an orthorhombic crystal (with the simple lattice), the residual 2D symmetry will be that of a rectangular unit cell with sides a and b, whereas for the case of a tetragonal crystal (with the simple lattice), the symmetry will be that of a square unit cell with sides a.

Since in the k_z direction, one can expand the function $f(\mathbf{k})$ in the form

$$f(\mathbf{k}_t,k_z)=\sum_M \phi^{(M)}(\mathbf{k}_t)e^{ik_zMd},\quad M=0,\pm1,\pm2,\pm3,\ldots$$
$$=\phi^{(0)}(\mathbf{k}_t)+\sum_{M=1}^{\infty}\{[\phi^{(M)}(\mathbf{k}_t)+\phi^{(-M)}(k_t)]\cos Mk_zd+i[\phi^{(M)}(\mathbf{k}_t)-\phi^{(-M)}(\mathbf{k}_t)]\sin Mk_zd\}, \tag{29}$$

the basis functions for expanding it as a function of k_z can be taken to be

$$\psi_{\Gamma^{(z)}}(k_z)\sim 1,\cos k_zd,\sin k_zd,\ldots \tag{30}$$

as classified in Table I. Since the coefficients with higher values of M involve overlaps of spatial functions in distant unit cells, we can keep only terms up to $|M|=1$. For expanding functions $\phi(\mathbf{k}_t)$ in layered crystals, the basis functions can be constructed by using the expansion

$$\phi(\mathbf{k}_t)=\sum_{\{R_L\}}\phi(\mathbf{R}_L)e^{i\mathbf{k}_t\cdot\mathbf{R}_L}=\sum_{\Gamma^{(2)}}\phi_{\Gamma^{(2)}}\psi_{\Gamma^{(2)}}(\mathbf{k}_t), \tag{31}$$

where one has to regroup the plane waves $e^{i\mathbf{k}_t\cdot\mathbf{R}_L}$ involving different two-dimensional direct lattice vectors $\mathbf{R}_L$ to transform as each of the IRR's $\Gamma^{(2)}$ of the residual two-dimensional point group. For the rectangular lattice, $\mathbf{R}_L=ma\hat{x}+nb\hat{y}$, and for the square lattice $\mathbf{R}_L=ma\hat{x}+na\hat{y}$; $m,n=0,\pm1,\pm2,\ldots$. In the two-dimensional residual point-group symmetry of a square corresponding to the 3D simple tetragonal case (D_{4h}), which is isomorphic to the group C_{4v}, there are eight elements, h_1, h_{14}, h_{26}, h_{37}, $h_4=I_2h_1$, $h_{15}=I_2h_{14}$, $h_{27}=I_2h_{26}$, $h_{40}=I_2h_{37}$, as defined by Kovalev,[11] where $I_2=C_2$ is the two-dimensional ''inversion'' operation in which $k_x\rightarrow-k_x$, $k_y\rightarrow-k_y$. In the two-dimensional residual symmetry point group (of rectangular unit cell) corresponding to the 3D simple orthorhombic case (D_{2h}), one has only four elements, h_1, h_{26}, $h_4=I_2h_1$, $h_{27}=I_2h_{26}$. The complete IRR's for both these residual symmetry groups are given in Tables II and III. For completeness, these tables also define the group elements h_i by listing below each one the resulting coordinates to which it transforms when it acts on the reciprocal space coordinate vector (k_x,k_y). Starting from the plane-wave expansion (31), and following the standard procedure, one can then construct the basis functions for each IRR for these 2D layer symmetries. They are also listed in the last column of Tables II and III, for these 2D symmetries under consideration.

TABLE I. Basis functions for k_z expansion.

IRR	Basis functions ($M=0,1,2,\ldots$)
$\Gamma_g^{(z)}$	$\psi_g^{(z)M}=\cos Mk_zd$:1,cos$k_zd,\ldots$
$\Gamma_u^{(z)}$	$\psi_u^{(z)M}=\sin Mk_zd$:sin$k_zd,\ldots$

For the spin-singlet pairing, one may obtain three-dimensional even-parity basis functions for the layered crystal by combining the even planar $\Gamma_g^{(2)}$ representations with

TABLE II. Irreducible representations and basis functions for 2D square lattice symmetry, C_{4v} (corresponding to 3-d simple tetragonal D_{4h}).

IRR	h_1 (k_x,k_y)	h_{14} $(-k_y,k_x)$	h_{26} $(-k_x,k_y)$	h_{37} (k_y,k_x)	h_4 $(-k_x,-k_y)$	h_{15} $(k_y,-k_x)$	h_{27} $(k_x,-k_y)$	h_{40} $(-k_y,-k_x)$	Basis functions $(m,n=0,1,2,\ldots)$
$\Gamma_{1g}^{(2\text{tet})}(A_{1g})$ $\sim(1,k_x^2+k_y^2)$	1	1	1	1	1	1	1	1	$\psi_{1g}^{(2\text{tet})mn}$ $=\cos mk_xa\,\cos nk_ya$ $+\cos nk_xa\,\cos mk_ya$ (s-wave like)
$\Gamma_{2g}^{(2\text{tet})}(A_{2g})$ $\sim k_xk_y(k_x^2-k_y^2)$	1	1	-1	-1	1	1	-1	-1	$\psi_{2g}^{(2\text{tet})mn}$ $=\sin mk_xa\,\sin nk_ya$ $-\sin nkxa\,\sin mkya$
$\Gamma_{3g}^{(2\text{tet})}(B_{1g})$ $\sim k_x^2-k_y^2$	1	-1	1	-1	1	-1	1	-1	$\psi_{3g}^{(2\text{tet})mn}$ $=\cos mk_x\,\cos nk_ya$ $-\cos nk_xa\,\cos k_ya$ ($d_{k_x^2-k_y^2}$-wave like)
$\Gamma_{4g}^{(2\text{tet})}(B_{2g})$ $\sim k_xk_y$	1	-1	-1	1	1	-1	-1	1	$\psi_{4g}^{(2\text{tet})mn}$ $=\sin mk_xa\,\sin nk_ya$ $+\sin nk_xa\,\sin mk_ya$ ($d_{k_xk_y}$-wave like)
$\Gamma_{5u}^{(2\text{tet})}(E_u)$ $\{k_x,k_y\}$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}0&-1\\1&0\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}0&1\\1&0\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}0&1\\-1&0\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}0&-1\\-1&0\end{pmatrix}$	$\{\psi_{5up_1}^{(2\text{tet})mn},\psi_{5up_2}^{(2\text{tet})mn}\}$ $=\{\sin mk_xa\,\cos nk_ya$ $\mp\sin nk_xa\,\cos mk_ya,$ $\mp\cos mk_xa\,\sin nk_ya$ $+\cos nk_xa\,\sin mk_ya\}$ $p=1,2\Rightarrow\mp$

the even $\Gamma_g^{(z)}$, and the odd planar $\Gamma_u^{(2)}$ representations with the odd $\Gamma_u^{(z)}$. In other words, for symmetric functions $f(\mathbf{k})=f(-\mathbf{k})$, one can use the following three-dimensional basis functions for its expansion in layered tetragonal and orthorhombic systems:

Tetragonal:

$$\psi_{Lg}^{(2\text{tet})mn}(k_x,k_y)\psi_g^{(z)M}(k_z),\psi_{5upq}^{(2\text{tet})mn}(k_x,k_y)\psi_u^{(z)M}(k_z);\ [\psi_\mu^{(3)}(\mathbf{k})]$$

$$L=1,2,3,4;\quad m,n,M=0,1,2,\ldots,\quad p,q=1,2, \tag{32}$$

Orthorhombic

$$\psi_{Lg}^{(2\text{orth})mn}(k_x,k_y)\psi_g^{(z)M}(k_z),\psi_{Lu}^{(2\text{orth})mn}(k_x,k_y)\psi_u^{(z)M}(k_z);\ [\psi_\mu^{(3)}(\mathbf{k})]$$

$$L=1,2;\quad m,n,M=0,1,2,\ldots, \tag{33}$$

where these functions are defined in the last column of Tables I–III.

It should be emphasized here that although the basis functions as shown in the above equations form an orthogonal set in each case if one integrates over all $\mathbf{k}$ in the Brillouin zone (BZ), one cannot take advantage of this property fully even while solving the linear gap equation for $\underline{\Delta}(\mathbf{k})$, because the integration is restricted through Fermi factors. For a layered crystal, with a widely open BZ in the k_z direction, whereas

TABLE III. Irreducible representations and basis functions for 2D rectangular lattice symmetry (corresponding to 3D-orthorhombic D_{2h}).

IRR	h_1 (k_x,k_y)	h_{26} $(-k_x,k_y)$	h_4 $(-k_x,-k_y)$	h_{27} $(k_x,-k_y)$	Basis functions $m,n=0,1,2,\ldots$
$\Gamma_{1g}^{(2)}$ $\sim(1,k_x^2,k_y^2)$	1	1	1	1	$\psi_{1g}^{(2\text{ orth})mn}$ $=\cos mk_xa\,\cos nk_yb$
$\Gamma_{2g}^{(2)}$ $\sim k_xk_y$	1	-1	1	-1	$\psi_{2g}^{(2\text{ orth})mn}$ $=\sin mk_xa\,\sin nk_yb$
$\Gamma_{1u}^{(2)}$ $\sim k_y$	1	1	-1	-1	$\psi_{1u}^{(2\text{ orth})mn}$ $=\cos mk_xa\,\sin nk_yb$
$\Gamma_{2u}^{(2)}$ $\sim k_x$	1	-1	-1	1	$\psi_{2u}^{(2\text{ orth})mn}$ $=\sin mk_xa\,\cos nk_yb$

TABLE IV. Forms for two-dimensional basis functions in cylindrical coordinates.

Basis functions for 2D layer of simple tetragonal lattice		
$A_{1g}(\sim 1, k_x^2+k_y^2)$	:	$1,(\cos k_x a+\cos k_y a),\cos k_x a\,\cos k_y a,\ldots$ (s-wave like)
$\psi_{1g}^{(2\text{tet})}(\mathbf{k}_t)$	$\sim$	$1, f_0(k_t a)+f_4(k_t a)\cos 4\phi+f_8(k_t a)\cos 8\phi+\cdots$
$B_{1g}[\sim(k_x^2-k_y^2)]$	:	$(\cos k_x a-\cos k_y a),(\cos 2k_x a-\cos 2k_y a),\ldots$ ($d_{k_x^2-k_y^2}$-like)
$\psi_{3g}^{(2\text{tet})}(\mathbf{k}_t)$	$\sim$	$f_2(k_t a)\cos 2\phi+f_6(k_t a)\cos 6\phi+\cdots$
$B_{2g}(\sim k_x k_y)$	:	$\sin k_x a\,\sin k_y a,(\sin 2k_x a\,\sin k_y a+\sin k_x a\,\sin 2k_y a),\ldots$ (d_{xy}-like)
$\psi_{4g}^{(2\text{tet})}$	$\sim$	$f_2'(k_t a)\sin 2\phi+f_6'(k_t a)\sin 6\phi+\cdots$
$A_{2g}[\sim k_x k_y(k_x^2-k_y^2)]$	:	$(\sin 2k_x a\,\sin k_y a-\sin k_x a\,\sin 2k_y a),\ldots$
$\psi_{2g}^{(2\text{tet})}$	$\sim$	$f_4'(k_t a)\sin 4\phi+f_8'(k_t a)\sin 8\phi+\cdots$
$\Gamma_{5u}^{(2\text{tet})}(\sim k_x, k_y)$	:	$\sin k_x a,\sin k_y a,\ldots$
$\psi_{5u}^{(2\text{tet})}$	$\sim$	$f_1(k_t a)\cos\phi+f_3(k_t a)\cos 3\phi+\cdots$, $f_1'(k_t a)\sin\phi+f_3'(k_t a)\sin 3\phi+\cdots$
Basis functions for 2D layer of simple orthorhombic lattice		
$\Gamma_{1g}^{(2)}(\sim 1, k_x^2, k_y^2)$	:	$1,\cos k_x a,\cos k_y b,\cos k_x a\,\cos k_y b,\ldots$ $\rightarrow$ (Mixed $A_{1g}+B_{1g}$ of tetragonal system)
$\psi_{1g}^{(2\text{orth})}(\mathbf{k}_t)$	$\sim$	$1,\chi_0(k_t)+\chi_2(k_t)\cos 2\phi+\chi_4(k_t)\cos 4\phi+\cdots$
$\Gamma_{2g}^{(2)}(\sim k_x k_y, k_x^3 k_y, k_x k_y^3)$	:	$\sin k_x a\,\sin k_y b,\sin 2k_x a\,\sin k_y b,\sin k_x a\,\sin 2k_y b,\ldots$ $\rightarrow$ (Mixed $A_{2g}+B_{2g}$ of tetragonal system)
$\psi_{2g}^{(2\text{orth})}(\mathbf{k}_t)$	$\sim$	$\chi_2'(k_t)\sin 2\phi+\chi_4'(k_t)\sin 4\phi+\cdots$
$\Gamma_{1u}^{(2)}(\sim k_y)$	:	$\sin k_y b,\sin k_y b\,\cos k_x a,\ldots$ $\rightarrow$ (deg. $\Gamma_{5u}^{(2\text{tet})}$ of tetragonal)
$\psi_{1u}^{(2\text{orth})}(\mathbf{k}_t)$	$\sim$	$\chi_1'(k_t)\sin\phi+\chi_3'(k_t)\sin 3\phi+\cdots$
$\Gamma_{2u}^{(2)}(\sim k_x)$	:	$\sin k_x a,\sin k_x a\,\cos k_y b,\ldots$ $\rightarrow$ (deg. $\Gamma_{5u}^{(2\text{tet})}$ of tetragonal)
$\psi_{2u}^{(2\text{orth})}(\mathbf{k}_t)$	$\sim$	$\chi_1(k_t)\cos\phi+\chi_3(k_t)\cos 3\phi+\cdots$

the integration over k_z, for any reasonable values of the carrier density, is over the full BZ, $-\pi/d \leq k_z \leq \pi/d$, the integrations over k_x, k_y do not cover the full BZ in the reciprocal-layer plane. In view of this, it is more convenient to use the cylindrical coordinates k_t, ϕ, and k_z, to take advantage of an additional orthogonality condition related to the integration over ϕ, with

$$k_x = k_t\cos\phi, \quad k_y = k_t\sin\phi, \quad k_z = k_z, \quad 0 \leq \phi \leq 2\pi. \tag{34}$$

In fact, for integrations near the Fermi surface, one can further transform the remaining third variable k_t to a suitable energy variable ξ. The two-dimensional basis functions for the tetragonal and orthorhombic systems can be rewritten in terms of the variables k_t and ϕ, instead of k_x and k_y, by using the Bessel-function ($J_m(z)$) expansions[12]

$$\cos k_x a = J_0(k_t a) - 2J_2(k_t a)\cos 2\phi + 2J_4(k_t a)\cos 4\phi - \cdots, \tag{35}$$

$$\cos k_y b = J_0(k_t b) + 2J_2(k_t b)\cos 2\phi + 2J_4(k_t b)\cos 4\phi + \cdots, \tag{36}$$

$$\sin k_x a = 2J_1(k_t a)\cos\phi - 2J_3(k_t a)\cos 3\phi + 2J_5(k_t a)\cos 5\phi - \cdots, \tag{37}$$

$$\sin k_y b = 2J_1(k_t a)\sin\phi + 2J_3(k_t b)\sin 3\phi + 2J_5(k_t b)\sin 3\phi + \cdots. \tag{38}$$

More explicitly, one can rewrite in terms of ϕ the forms of 2D basis functions relevant to tetragonal and orthorhombic layered crystals, as shown in Table IV. We also give in this table some of the simpler basis functions in k_x, k_y variables, for easy identification.

Note that for the orthorhombic case, one does not have any pure $d_{k_x^2-k_y^2}$ or $d_{k_x k_y}$-like basis functions of the spherical symmetry, which are related, respectively, to B_{1g} and B_{2g} symmetries of the tetragonal system. They are always mixed with extended s-wave-like (A_{1g}) or A_{2g}-like basis functions. However, a pure isotropic s-wave-like basis function (1) is always possible in each case.

IV. PROBLEMS OF ONE AND TWO LAYERS PER UNIT CELL

To apply the symmetry considerations to the spin-singlet theory in layered crystals, in this section we consider the case of $N=1$ as well as $N=2$ layers per unit cell. This will illustrate the application of our method to both the situations in which either only intralayer pairing is possible ($N=1$) or both intralayer and interlayer pairings are allowed ($N=2$).

A. The $N=1$ problem

The problem of one layer ($N=1$) per unit cell is simplest to consider because in this case we have only intralayer pairing, with a nonmatrix order parameter $\Delta_{11}(\mathbf{k})\equiv\Delta(\mathbf{k})$, which is also the quasiparticle energy E_g (at FS) in the superconducting state. Here, $g(k)=(i\omega_m-\xi)^{-1}$, $\xi=\xi(\mathbf{k})=\epsilon(\mathbf{k}_t)-2t'\cos k_z d-\mu$, $g^{\rm trans}(-k)=(-i\omega_m-\xi)^{-1}$. If one further assumes that $V(k,k')$ and $\Delta(k')$ are independent of frequencies, except for the frequency cutoffs, the usual summation over $\omega_{m'}$ in Eq. (18) then leads to the well-known BCS gap equation

$$\Delta(\mathbf{k})=-\sum_{\mathbf{k}'} V(\mathbf{k},\mathbf{k}')\Delta(\mathbf{k}')T(\beta,E'), \tag{39}$$

$$T(\beta,E')\equiv\tanh(\beta E'/2)/2E', \quad \beta=1/k_BT,$$

$$E'=E(\mathbf{k}')=[\xi^2(\mathbf{k}')+\Delta^2(\mathbf{k}')]^{1/2}. \tag{40}$$

Near $T=T_c$, the linearized form of the BCS equation is immediately obtained by replacing E' by $\xi'=\xi(\mathbf{k}')$ in the above equation.

In terms of the three-dimensional basis functions given in Eqs. (32) and (33) for tetragonal and orthorhombic systems, which we label by $\psi_\mu^{(3)}(\mathbf{k})$, $\mu=1,2,\ldots$, the interaction function $V(\mathbf{k},\mathbf{k}')$ can be expanded in the form

$$V(\mathbf{k},\mathbf{k}')=\sum_\mu\sum_\nu V^{(\mu,\nu)}\psi_\mu^{(3)}(\mathbf{k})\psi_\nu^{(3)}(\mathbf{k}'), \quad V^{(\mu,\nu)}=V^{(\nu,\mu)}. \tag{41}$$

The solution for the order parameter, which is also the gap function $E_g(\mathbf{k})$, has then the general form

$$\begin{aligned}\Delta(\mathbf{k})&=\sum_\mu \Delta^{(\mu)}\psi_\mu^{(3)}(\mathbf{k})\\ &\simeq\sum_{\Gamma_g}[\Delta^{(0)\Gamma_g}\psi_{\Gamma_g}^{(2)}(\mathbf{k}_t)+\Delta^{(1)\Gamma_g}\psi_{\Gamma_g}^{(2)}(\mathbf{k}_t)\cos k_z d]\\ &\quad+\sum_{\Gamma_u}\Delta^{(1)\Gamma_u}\psi_{\Gamma_u}^{(2)}(\mathbf{k}_t)\sin k_z d,\end{aligned} \tag{42}$$

where $\psi_\Gamma^{(2)}(\mathbf{k}_t)$ are basis functions of the corresponding two-dimensional representations, given in Table IV. Near $T=T_c$, when one is solving the linear gap equation for finding T_c, it is possible to assume that only one two-dimensional IRR in the summation in Eq. (42), which gives maximum T_c, is relevant. In Ref. 10, we have analyzed a part of this problem in detail to explore the mixing of the s-wave-like and d-wave like symmetries in the possible solutions and the corresponding T_c, in which we restricted the energy integration over ξ' close to the FS. It also included an approximate analysis of the more general problem of N layers per unit cell in which only intralayer pairings were allowed and the interlayer single-particle tunneling within each unit cell was neglected. We showed that in the orthorhombic system, it is not possible to obtain a planar $d_{k_x^2-k_y^2}$-like (B_{1g}) solution ($\sim\cos 2\phi$), without any admixture of the planar s-wave-like (A_{1g}) solution ($\sim f_0+f_1\cos 4\phi$). Similarly, it is easy to show that one does not have a $d_{k_xk_y}$-like (B_{2g}) solution ($\sim\sin 2\phi$) without the admixture of A_{2g}-like solution ($\sim\sin 4\phi$) in the orthorhombic system. Of course, there are additional correction terms in the gap function proportional to $\cos k_z d$, as shown in Eq. (42). Because of the orthogonality of functions, $\cos m\phi'$, $\cos n\phi'$, $\sin m\phi'$, $\sin n\phi'$, etc., when integrated over ϕ' in the gap equation, and because of the general structure of the basis functions for the orthorhombic and tetragonal systems, as shown in terms of these functions in Table IV, the above result is valid more generally, and one does not need the approximation to restrict the energy integrations close to the FS. In the orthorhombic case, the possible solutions are of the form

$$\begin{aligned}\Delta(\mathbf{k})&=\Delta^{(0)0}+\Delta^{(1)0}\cos k_z d;[\Delta^{(0)0}(k_t)+\Delta^{(0)1}(k_t)\cos 2\phi+\Delta^{(0)2}(k_t)\cos 4\phi+\cdots]\\ &\quad+[\Delta^{(1)0}(k_t)+\Delta^{(1)1}\cos 2\phi+\Delta^{(1)2}\cos 4\phi+\cdots]\cos k_z d;\cdots\ \cdots\ \cdots;\text{etc.},\end{aligned} \tag{43}$$

which can be written down directly from the possible two-dimensional basis functions $\psi_\Gamma^{(2\ \rm orth)}(\mathbf{k}_t)$ given in Table IV. Similarly, the form of possible solutions for $\Delta(\mathbf{k})$ in the tetragonal system can be immediately obtained by using the form of the basis functions $\psi_\Gamma^{(2\ \rm tet)}(\mathbf{k}_t)$ given in Table IV and Eq. (42). Here, planar $d_{k_x^2-k_y^2}$-like or $d_{k_xk_y}$-like pairing symmetries can occur without any admixture of A_{1g} or A_{2g} symmetry. Next, we consider the problem of two layers per unit cell ($N=2$), where both intralayer and interlayer pairings are possible.

B. The $N=2$ problem

In the case of two layers per unit cell, we have to deal with 2×2 matrices $\underline{g}(k)$, $\underline{g}^{\rm trans}(-k)$ and $\underline{\Delta}(k)$. Here, in our layer representation the normal-state inverse Green function for two layers per unit cell can be taken to be of the form

$$\underline{g}^{-1}(k)=\begin{pmatrix} i\omega_m-\tilde{\xi}_1 & -|t|e^{i\eta}\\ -|t|e^{-i\eta} & i\omega_m-\tilde{\xi}_2\end{pmatrix},$$

$$[\underline{g}^{\rm trans}(-k)]^{-1}=\begin{pmatrix} -i\omega_m-\tilde{\xi}_1 & -|t|e^{i\eta}\\ -|t|e^{-i\eta} & -i\omega_m-\tilde{\xi}_2\end{pmatrix}, \tag{44}$$

where

$$\tilde{\xi}_{1,2}(\mathbf{k})=\tilde{\epsilon}_{1,2}(\mathbf{k})-\mu=\epsilon_{1,2}(\mathbf{k}_t)-2t'_{1,2}\cos k_z d-\mu, \tag{45}$$

$$t\equiv t(\mathbf{k})=|t(\mathbf{k})|e^{i\eta(\mathbf{k})}=t_{12}(\mathbf{k}_t)+t'_{12}(\mathbf{k}_t)\exp(ik_z d), \tag{46}$$

$$\tan\eta = t'_{12}\sin k_z d/(t_{12}+t'_{12}\cos k_z d),$$

$$\eta(-\mathbf{k}) = -\eta(\mathbf{k}) = -\eta. \tag{47}$$

In this layer representation, if we ignore the frequency dependence of the order parameter (except for the frequency cutoff), it has the general form

$$\underline{\Delta}(\mathbf{k}) = \begin{pmatrix} \Delta_{11}(\mathbf{k}) & \Delta_{12}(\mathbf{k}) \\ \Delta_{21}(\mathbf{k}) & \Delta_{22}(\mathbf{k}) \end{pmatrix}, \tag{48}$$

where we may assume Δ_{11} and Δ_{22} to be real symmetric functions of $\mathbf{k}$ and $\Delta_{21}(\mathbf{k}) = \Delta_{12}(-\mathbf{k}) = \Delta^*_{12}(\mathbf{k})$. In terms of real functions $\Delta_\perp(\mathbf{k})$ and $\theta(\mathbf{k})$, one may assume

$$\Delta_{12}(\mathbf{k}) = \Delta_\perp(\mathbf{k}) e^{i\theta(\mathbf{k})}, \quad \Delta_\perp(-\mathbf{k}) = \Delta_\perp(\mathbf{k}) \equiv |\Delta_{12}(\mathbf{k})|,$$

$$\theta(-\mathbf{k}) = -\theta(\mathbf{k}). \tag{49}$$

In view of the nondiagonal form for both $\underline{g}$ and $\underline{\Delta}$ in the layer representation, the general consideration of this problem for obtaining the gap equation for $\underline{\Delta}(\mathbf{k})$ from Eq. (18), after performing the summation over $\omega_{m'}$, and for finding the quasiparticle excitation energies $E(\mathbf{k})$ by determining the zeroes of the determinant of the inverse Green function $G^{-1}(\mathbf{k}, i\omega_m = E)$ from Eq. (17), is somewhat tedious. Instead, as discussed in I, one may take advantage of the so-called α representation in which $\underline{g}(k)$ and $\underline{g}^{\text{trans}}(-k)$ are diagonal. The unitary matrix $S(\mathbf{k})$ which diagonalizes these matrices are given by

$$\underline{S}^{-1}(\mathbf{k})\underline{g}(k)\underline{S}(\mathbf{k}) = \underline{g}^{(\alpha)}(k),$$

$$\underline{S}^{-1}(\mathbf{k})\underline{g}^{\text{trans}}(-k)\underline{S}(k) = \underline{g}^{(\alpha)\text{trans}}(-k), \tag{50}$$

$$\underline{S}(\mathbf{k}) = \begin{pmatrix} \cos\Psi & -e^{i\eta}\sin\Psi \\ e^{-i\eta}\sin\Psi & \cos\Psi \end{pmatrix},$$

$$\underline{S}^{-1}(\mathbf{k}) = \begin{pmatrix} \cos\Psi & e^{i\eta}\sin\Psi \\ -e^{-i\eta}\sin\Psi & \cos\Psi \end{pmatrix}, \tag{51}$$

$$\underline{g}^{(\alpha)}(k) = \begin{pmatrix} (i\omega_m - \xi_1)^{-1} & 0 \\ 0 & (i\omega_m - \xi_2)^{-1} \end{pmatrix}, \tag{52}$$

$$\underline{g}^{(\alpha)\text{trans}}(-k) = \begin{pmatrix} -(i\omega_m + \xi_1)^{-1} & 0 \\ 0 & -(i\omega_m + \xi_2)^{-1} \end{pmatrix}, \tag{53}$$

$$\xi_{1,2}(\mathbf{k}) = \tfrac{1}{2}[\tilde{\xi}_1(\mathbf{k}) + \tilde{\xi}_2(\mathbf{k})] \pm \tfrac{1}{2}[[\tilde{\xi}_1(\mathbf{k}) - \tilde{\xi}_2(\mathbf{k})]^2 + 4|t(\mathbf{k})|^2]^{1/2}, \tag{54}$$

$$\tan 2\Psi = 2|t(\mathbf{k})|/[\tilde{\xi}_1(\mathbf{k}) - \tilde{\xi}_2(\mathbf{k})], \quad \text{with} \quad \xi_1 \neq \xi_2. \tag{55}$$

In this representation, $\underline{\Delta}^{(\alpha)}$ has the form

$$\underline{\Delta}^{(\alpha)}(\mathbf{k}) = \underline{S}^{-1}(\mathbf{k})\underline{\Delta}(\mathbf{k})\underline{S}(\mathbf{k}) = \begin{pmatrix} \Delta^{(\alpha)}_{11}(\mathbf{k}) & \Delta^{(\alpha)}_{12}(\mathbf{k}) \\ \Delta^{(\alpha)}_{21}(\mathbf{k}) & \Delta^{(\alpha)}_{22}(\mathbf{k}) \end{pmatrix} \tag{56}$$

with

$$\Delta^{(\alpha)}_{11} = [\tfrac{1}{2}(\Delta_{11}+\Delta_{22}) + \tfrac{1}{2}(\Delta_{11}-\Delta_{22})\cos 2\Psi + |\Delta_{12}|\sin 2\Psi\ \cos(\theta-\eta)], \tag{57}$$

$$\Delta^{(\alpha)}_{12} = e^{i\eta}[-\tfrac{1}{2}(\Delta_{11}-\Delta_{22})\sin 2\Psi + |\Delta_{12}|\cos 2\Psi\ \cos(\theta-\eta) + i|\Delta_{12}|\sin(\theta-\eta)], \tag{58}$$

$$\Delta^{(\alpha)}_{21} = \Delta^{(\alpha)*}_{12}, \tag{59}$$

$$\Delta^{(\alpha)}_{22} = [\tfrac{1}{2}(\Delta_{11}+\Delta_{22}) - \tfrac{1}{2}(\Delta_{11}-\Delta_{22})\cos 2\Psi - |\Delta_{12}|\sin 2\Psi\cos(\theta-\eta)]. \tag{60}$$

Note that even for a system with two equivalent layers, where $\tilde{\xi}_1 = \tilde{\xi}_2$, so that $\Psi = \pi/4$, $\Delta_{22} = \Delta_{11} = \Delta$, $\Delta^{(\alpha)}(\mathbf{k})$ is diagonal only if $t(\mathbf{k})$ and $\Delta_{12}(\mathbf{k})$ are real functions (i.e., $\theta = \eta = 0$) or if accidentally $\theta = \eta$. In such special cases, one can write down the BCS equations for two branches separately, each one being similar to Eq. (39), where quasiparticle energies in these two branches are given by $E_{1,2}(\mathbf{k}) = [\xi^2_{1,2}(\mathbf{k}) + E^2_{g1,2}]^{1/2}$, where $E_{g1} = \Delta(\mathbf{k}) + \Delta_\perp(\mathbf{k})$, $E_{g2} = \Delta(\mathbf{k}) - \Delta_\perp(\mathbf{k})$. However, these expressions are not simple in general.

For the more general case, in which $t(\mathbf{k}) = |t|e^{i\eta}$ and $\Delta_{12}(\mathbf{k}) = |\Delta_{12}|e^{i\theta}$ are complex, the problem of finding T_c and the zeroes of the determinant of $\underline{G}^{-1}(\mathbf{k}, i\omega_m = E)$ to obtain an expression for the quasiparticle energy $E(\mathbf{k})$ can still be solved more easily by using the α representation in which $\underline{g}$ is diagonal. This method was used by us in I where we had ignored the $\mathbf{k}_t$ dependence of $\underline{\Delta}$. Working in the α representation, if we ignore the frequency dependence of $\underline{\Delta}^{(\alpha)}$ and $\underline{V}^{(2)}$ (except for the cutoffs) one can perform the summation over $\omega_{m'}$ in the linear gap Eq. (19) to obtain the following equation to determine T_c:

$$\Delta^{(\alpha)}_{\alpha_1\alpha_2} = -\sum_{\mathbf{k}'} \sum_{\alpha_3\alpha_4} V^{(\alpha)}_{\alpha_1\alpha_2,\alpha_3\alpha_4}(\mathbf{k},\mathbf{k}') A_{\alpha_3\alpha_4}(\mathbf{k}'), \tag{61}$$

$$\underline{A}(\mathbf{k}') = \begin{pmatrix} \Delta^{(\alpha)}_{11}(\mathbf{k}')T_{11}(\beta_c,\xi'_1,\xi'_1) & \Delta^{(\alpha)}_{12}(\mathbf{k}')T_{12}(\beta_c,\xi'_1,\xi'_2) \\ \Delta^{(\alpha)}_{21}(\mathbf{k}')T_{21}(\beta_c,\xi'_2,\xi'_1) & \Delta^{(\alpha)}_{22}(\mathbf{k}')T_{22}(\beta_c,\xi'_2,\xi'_2) \end{pmatrix}, \tag{62}$$

$$T_{ij}(\beta,\xi_i,\xi_j) \equiv \frac{[\tanh(\beta\xi_i/2) + \tanh(\beta\xi_j/2)]}{2(\xi_i+\xi_j)}, \tag{63}$$

$$V^{(\alpha)}_{\alpha_1\alpha_2,\alpha_3\alpha_4}(\mathbf{k},\mathbf{k}')=\sum_{J_1J_2}\sum_{J_3J_4} S^{-1*}_{\alpha_1J_1}(\mathbf{k})S^{-1}_{\alpha_2J_2}(\mathbf{k})V_{J_1J_2,J_3J_4}(\mathbf{k},\mathbf{k}')S^{*}_{J_3\alpha_3}(\mathbf{k}')S_{J_4\alpha_4}(\mathbf{k}'). \tag{64}$$

Here, $T_{ij}=T_{ji}$ and $\Delta^{(\alpha)}_{12}(\mathbf{k})=\Delta^{(\alpha)*}_{21}(\mathbf{k})$. To find the nature of T_c, one can again use the same method as in I, by using a suitable parametrization of the interaction function $\underline{\underline{V}}$.

Coming back to the layer representation, from the roots of the determinantal equation

$$\det|\underline{G}^{-1}(\mathbf{k},E)|=\det\{\underline{g}^{-1}(k)[\underline{I}+\underline{g}(\mathbf{k},E)\underline{\Delta}(\mathbf{k})\underline{g}^{\mathrm{trans}}(-\mathbf{k},-E)\underline{\Delta}(\mathbf{k})]=0, \tag{65}$$

we find the most general expression for the quasiparticle energy (for $N=2$) in the form

$$E^2_{1,2}(\mathbf{k})=\tfrac{1}{2}[\xi^2_1+\xi^2_2+\Delta^2_{11}+\Delta^2_{22}+2|\Delta_{12}|^2]\pm\tfrac{1}{2}\,[\{\xi^2_1-\xi^2_2+(\Delta_{11}+\Delta_{22})[(\Delta_{11}-\Delta_{22})\cos2\Psi+2|\Delta_{12}|\sin\Psi\,\cos(\theta-\eta)]\}^2$$
$$+\{[(\Delta_{22}-\Delta_{11})\sin2\Psi+2|\Delta_{12}|\cos2\Psi\cos(\theta-\eta)]^2+4|\Delta_{12}|^2\sin^2(\theta-\eta)\}\{(\xi_1-\xi_2)^2+(\Delta_{11}+\Delta_{22})^2\}]^{1/2}. \tag{66}$$

Note that for the case of two equivalent layers ($\Psi=\pi/4$), this goes over to the special decoupled form $E^2_{1,2}(\mathbf{k})=\xi^2_{1,2}(\mathbf{k})+[\Delta(\mathbf{k})\pm\Delta_\perp(\mathbf{k})]^2$, when $\Delta_{11}=\Delta_{22}\equiv\Delta(\mathbf{k})$, $|\Delta_{12}(\mathbf{k})|\equiv\Delta_\perp(\mathbf{k})$, only if $\Delta_{12}(\mathbf{k})$ and $t(\mathbf{k})$ are real (i.e., $\theta=\eta=0$). One can immediately obtain the form of the energy gap function $E_g(\mathbf{k})$, by putting $\xi_1=\xi_2=0$ in the above expression. However, there is no need to follow this tedious route to find $E_g(\mathbf{k})$, since we are primarily interested in this paper in the symmetry aspects of the gap function $E_g(\mathbf{k})$, i.e., in the quasiparticle energy the layer representation itself without using the α representation. For $N=2$, it implies

$$\det\begin{vmatrix}\Delta_{11}(\mathbf{k})\mp E_g & \Delta_\perp(\mathbf{k})e^{i\theta(\mathbf{k})}\\ \Delta_\perp(\mathbf{k})e^{-i\theta(\mathbf{k})} & \Delta_{22}(\mathbf{k})\mp E_g\end{vmatrix}=0. \tag{67}$$

Suppressing the overall sign in each case, this leads to the following expressions for the gap function in the two branches:

$$E_{g1,2}(\mathbf{k})=\tfrac{1}{2}\{(\Delta_{11}(\mathbf{k})+\Delta_{22}(\mathbf{k}))$$
$$\pm[(\Delta_{11}(\mathbf{k})-\Delta_{22}(\mathbf{k}))^2+4\Delta^2_\perp(k)]^{1/2}\}, \tag{68}$$

which reduces to the same form, $E_{g1,2}=\Delta(\mathbf{k})\pm\Delta_\perp(\mathbf{k})$, as obtained in the special case of real $t(\mathbf{k})$ and $\Delta_{12}(\mathbf{k})$, when $\Delta_{11}(\mathbf{k})=\Delta_{22}(\mathbf{k})=\Delta(\mathbf{k})$. However, in the general case one does not get simple decoupled forms for the quasiparticle energy away from the FS, if one examines Eq. (66). It may be noted from the expressions for $\Delta^{(\alpha)}_{\alpha_1\alpha_2}(\mathbf{k})$ given in Eqs. (56)–(60) that the form of $E_{g1,2}$ is exactly the same as given in Eq. (68), even in the α representation for $\Delta^{(\alpha)}$. Similarity transformation does not change the eigenvalues. In any case, as far as the gap function E_g at the FS in the two branches is concerned, we have the general result (68) for $N=2$ in the layer representation, where one has nonvanishing order parameters for both intralayer pairings and interlayer pairings. The intralayer functions $\Delta_{11}(\mathbf{k})$ and $\Delta_{22}(\mathbf{k})$ as well as interlayer functions $\Delta_\perp(\mathbf{k})$ are real and symmetric functions of $\mathbf{k}$. These functions can therefore be expanded in terms of the basis functions already discussed for the $N=1$ case. For equivalent layers, for real $\Delta_{11}(\mathbf{k})$ and $\Delta_{22}(\mathbf{k})$, intralayer order parameters can differ at most by a sign, $\Delta_{22}(\mathbf{k})=\pm\Delta_{11}(\mathbf{k})$, but interlayer order parameter $\Delta_\perp(\mathbf{k})$ need not have the same symmetry. For example, for a tetragonal system $\Delta_{11}(\mathbf{k})$ and $\Delta_{22}(\mathbf{k})$ can both have the $d_{k^2_x-k^2_y}$-like B_{1g} symmetry in the layer plane, but $\Delta_\perp(\mathbf{k})$ may have even an isotropic k_t-independent s-wave-like form of the A_{1g} symmetry. Note that in the presence of interlayer pairings, the nodes due to the zeroes in the intralayer order parameters alone will get shifted in the two branches of the energy gap function. In what follows, in the next section we will now apply our method to explore the symmetry of the gap functions in the general case of N layers per unit cell.

V. THE ENERGY-GAP FUNCTION AND ITS SYMMETRY FOR THE CASE OF N LAYERS PER UNIT CELL

As discussed in the last section, as N increases from 1 the general problem of N layers per unit cell becomes more and more difficult to handle in the presence of the complex single-particle tunneling matrix elements between the layers in a given unit cell. Only if this tunneling is very weak so that it can be neglected in the first approximation, in principle, can one then consider the case of general N-inequivalent layers per unit cell more easily. In such a case, $\underline{g}(k)$ and $\underline{g}^{\mathrm{trans}}(k)$ are diagonal, with $g_{JJ}(k)=(i\omega_m-\xi_J)^{-1}$, $g^{\mathrm{trans}}_{JJ}(-k)=-(i\omega_m+\xi_J)^{-1}$. Here, ξ_J is the single-particle energy for the layer J, which need not be equivalent. With the usual approximation regarding the frequency dependence of $\underline{\underline{V}}(k,k')$ and $\underline{\Delta}(k)$, the summation over $\omega_{m'}$ in Eq. (19) then leads to the generalized linear BCS gap equation

$$\Delta_{J_1J_2}(\mathbf{k})=-\sum_{\mathbf{k}'}\sum_{J_3J_4}V_{J_1J_2,J_3J_4}(\mathbf{k},\mathbf{k}')\Delta_{J_3J_4}(\mathbf{k}')$$
$$\times T_{J_3J_4}(\beta,\xi'_{J_3},\xi'_{J_4}), \tag{69}$$

$$T_{J_3J_4}(\beta,\xi'_{J_3},\xi'_{J_4})\equiv\frac{1}{2}\left[\frac{\tanh\beta\xi_{J_3}(\mathbf{k}')+\tanh\beta\xi_{J_4}(\mathbf{k}')}{\xi_{J_3}(\mathbf{k}')+\xi_{J_4}(\mathbf{k}')}\right]. \tag{70}$$

This includes both intralayer and interlayer pairings. In case one restricts to intralayer pairings only, with $\Delta_{J_1J_2}(\mathbf{k})=\Delta_{J_1}\delta_{J_1,J_2}$, the above equation simplifies further to the familiar form

$$\Delta_J(\mathbf{k}) = -\sum_{\mathbf{k}'} \sum_{J'} V_{J,J'}(\mathbf{k},\mathbf{k}')\Delta_{J'}(\mathbf{k}') \times \frac{\tanh[\xi_{J'}(\mathbf{k}')/2k_BT_c]}{2\xi_{J'}(\mathbf{k}')}, \tag{71}$$

where $V_{JJ,J'J'} \equiv V_{J,J'}$. The consideration of possible symmetries for $\Delta_J(\mathbf{k})$ and the expression for the corresponding T_c in this case has already been discussed by us earlier.[10]

As we have emphasized here in this paper, without making any of the above approximations regarding the tunneling matrix elements and interlayer order parameters, the symmetry of the gap function E_g can be analyzed in the most general case by diagonalizing the matrix $\underline{\Delta}$ in the layer representation. In other words, one has just to find the roots of the determinant

$$\det \begin{vmatrix} \Delta_{11}(\mathbf{k})-E_g & \Delta_{12}(\mathbf{k}) & \Delta_{13}(\mathbf{k}) & \cdots & \Delta_{1N}(\mathbf{k}) \\ \Delta_{12}^*(\mathbf{k}) & \Delta_{22}(\mathbf{k})-E_g & \Delta_{23}(\mathbf{k}) & \cdots & \Delta_{2N}(\mathbf{k}) \\ \Delta_{13}^*(\mathbf{k}) & \Delta_{23}^*(\mathbf{k}) & \Delta_{33}(\mathbf{k})-E_g & \cdots & \Delta_{3N}(\mathbf{k}) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \Delta_{1N}^*(\mathbf{k}) & \Delta_{2N}^*(\mathbf{k}) & \Delta_{3N}^*(\mathbf{k}) & \cdots & \Delta_{NN}(\mathbf{k})-E_g \end{vmatrix} = 0 \tag{72}$$

to obtain the N branches of $E_g(\mathbf{k})$. Here, $\Delta_{JJ}(\mathbf{k})$ may be taken to be real symmetric functions of $\mathbf{k}$, whereas the amplitudes of the off-diagonal elements are symmetric but the phases are antisymmetric functions of $\mathbf{k}$. The above general analysis simplifies considerably for the case in which diagonal elements $\Delta_{11}=\Delta_{22}=\cdots=\Delta(\mathbf{k})$, for equivalent N layers, and there are interlayer pairings only between the nearest-neighbor layers, with $\Delta_{J,J+1}(\mathbf{k})=\Delta_{12}(\mathbf{k})=\Delta_\perp(\mathbf{k})e^{i\theta(\mathbf{k})}$, $\Delta_{J+1,J}(\mathbf{k})=\Delta_{21}(\mathbf{k})=\Delta_\perp(\mathbf{k})e^{-i\theta(\mathbf{k})}$. The determinant in Eq. (72) in this case reduces to the form

$$\det \begin{vmatrix} x & e^{i\theta} & 0 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ e^{-i\theta} & x & e^{i\theta} & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ 0 & e^{-i\theta} & x & e^{i\theta} & \cdots & \cdots & \cdots & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & e^{-i\theta} & x \end{vmatrix} = 0, \tag{73}$$

where

$$x \equiv (\Delta(\mathbf{k})-E_g)/\Delta_\perp(\mathbf{k}). \tag{74}$$

For a given N, as a function on x the above determinant is a Chebyshev polynomial[12] $S_N(x)$ of order N which satisfies the recurrence relation

$$S_{N+1}(x) = xS_N(x) - S_{N-1}(x), \quad \text{with } S_0(x)=1, \quad S_1(x)=x. \tag{75}$$

Since the zeroes of the polynomial $S_N(x)$ are given by $2\cos[\pi p/(N+1)]$, $p=1,2,\ldots,N$, we immediately obtain the expression for E_g in all the N branches:

$$E_{gp}(\mathbf{k}) = \Delta(\mathbf{k}) - 2\Delta_\perp(\mathbf{k})\cos[\pi p/(N+1)], \quad p=1,2,\ldots,N. \tag{76}$$

This gives the correct results for $N=1$ and 2, already obtained in the last section, and it implies that as $N\to\infty$, the N branches of the gap function are bounded between $\Delta(\mathbf{k})-2\Delta_\perp(\mathbf{k})$ and $\Delta(\mathbf{k})+2\Delta_\perp(\mathbf{k})$. As already explained for the case of $N=2$ layers per unit cell, the symmetry of $E_{gp}(\mathbf{k})$ is determined by the possible symmetries of the real and symmetric intralayer and interlayer pairing functions $\Delta(\mathbf{k})$ and $\Delta_\perp(\mathbf{k})$, along with expression (58). These two functions need not correspond to the basis functions of the same IRR, listed in Table IV.

VI. CONCLUDING REMARKS

In the preceding sections, we have presented a first-principles analysis of possible symmetries of the superconducting order parameters $\Delta_{JJ'}(\mathbf{k}_t,k_z)$ and the corresponding quasiparticle energy gap function $E_g(\mathbf{k}_t,k_z)$ at the Fermi surface in high-T_c layered superconductors with either a simple orthorhombic or tetragonal unit cell. This has been done in terms of all possible irreducible representations and the corresponding basis functions, which are relevant to layered crystals in which the symmetry may be restricted to the lattice periodicity perpendicular to the layers for each layer in the unit cell, and the residual two-dimensional point-group symmetry of the planar unit cell in each layer along with its lattice periodicity in the (x,y)-layer plane. Our consideration clearly shows that many reported experimental observations[1] claiming planar $d_{k_x^2-k_y^2}$-like (B_{1g}) symmetry for the energy gap function in several high-T_c materials can only be approximate, for various reasons. First of all, in orthorhombic systems the planar $d_{k_x^2-k_y^2}$-like (B_{1g}) symmetry is always mixed with the s-wave-like (A_{1g}) symmetry of the corresponding tetragonal system. Also, in both orthorhombic as well as tetragonal systems, there is a possibility of a weak modulation of the energy gap function ($\sim\cos k_z d$) in the direction perpendicular to the reciprocal (k_x,k_y)-layer plane. In addition, for more than one layer per unit cell, in the presence of interlayer pairings we find that even in the tetragonal case it is not necessary to find a pure $d_{k_x^2-k_y^2}$-like (B_{1g}) symmetry with nodes at $k_x=\pm k_y$ for the corresponding gap functions $E_{gp}(\mathbf{k})$. The interlayer order parameters

$\Delta_{JJ'}(\mathbf{k})$, $J \neq J'$, which may not have the same symmetry as the intralayer pairing parameters $\Delta_{JJ}(\mathbf{k})$, always modify the structure of the energy gap function $E_g(\mathbf{k})$.

In view of the results obtained here, it may not be possible to determine the symmetry of $E_g(\mathbf{k})$ correctly, unless one obtains its full form experimentally[13] as a function of ϕ. If one can suppress the possible weak dependence of $E_g(\mathbf{k})$ on k_z, the experimental observations should first be fitted with a general form

$$E_g(\mathbf{k}) = \sum_{n=0}^{\infty} [A_n \cos n\phi + B_n \sin n\phi] \tag{77}$$

to determine the coefficients A_n and B_n, at least up to $n = 4$. Then, with the help of the basis functions for different IRR's as listed in Table IV, it would be possible to determine its symmetry. In particular, it is expected that in orthorhombic systems, with, e.g., dominant $d_{k_x^2 - k_y^2}$-like symmetry for $E_g(\mathbf{k})$, one may be able to fit most of the data with the form, $A_0 + A_2 \cos 2\phi + A_4 \cos 4\phi$, consistent with symmetry considerations.

In this paper, we have emphasized the role of the residual layer symmetry in exploring the form of the energy gap function $E_g(\mathbf{k})$ in layered high-T_c crystals. However, one may ask the question, why should we not analyze the symmetry in terms of the usual full three-dimensional representations of the crystal unit cell? The reason for advocating the route adopted here is that high-T_c cuprates are highly layered materials with almost two-dimensional dynamics for each layer. The interlayer tunneling matrix elements are quite weak, with a widely open Fermi surface in the k_z direction. In the layer-representation approach, one can even study the limiting case when this tunneling takes vanishing values. In such a case, when tunneling matrix elements become smaller than $k_B T_c$ and when there are no interlayer pairings, one will, of course, go over to the regime of ''intrinsic'' Josephson tunneling[9] between the ''independent'' superconducting layers in the unit cell, for which there is already experimental evidence[14] reported in the literature. We hope to discuss this relationship in a future publication. Another class of tunneling phenomena in a variety of junctions considered by Tanaka and co-workers[1] gives rise to mid-gap surface states due to the interface structure, which will exhibit strong anisotropy. These may be expected to display further structure due to interlayer coupling discussed in this paper. We expect that these effects will shed more light on the intrinsic anisotropy of pairing phenomena in high-T_c superconductors and we hope to address these issues in another publication. In any case, as long as the single-particle tunneling matrix elements remain small compared to μ, our formulation of the problem should be very good for layered materials, because it includes all the essential elements of the problem in such systems.

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[1] C. C. Tsuei, J. R. Kirtley, C. C. Chi, L. S. Yu-Jahnes, A. Gupta, T. M. Shaw, J. Z. Sun, and M. B. Ketchen, Phys. Rev. Lett. **72**, 593 (1994); J. R. Kirtley, C. C. Tsuei, J. Z. Sun, C. C. Chi, L. S. Yu-Jahnes, A. Gupta, M. Rupp, and M. B. Ketchen, Nature (London) **373**, 225 (1995); J. H. Miller, Jr., Q. Y. Ying, Z. G. Zon, N. Q. Fan, J. H. Xu, M. F. Davis, and J. C. Wolfe, Phys. Rev. Lett. **74**, 2347 (1995); M. R. Norman, M. Randeria, H. Ding, and J. C. Campuzana, Phys. Rev. B **52**, 15 017 (1995); D. A. Wollman, D. J. Van Harlingen, J. Giapintzakis, and D. M. Ginsberg, Phys. Rev. Lett. **74**, 797 (1995). For other experimental papers, see J. Phys. Chem. Solids **56**, 1645 (1995); **56**, 1783 (1995); **56**, 1797 (1995); **56**, 1841 (1995); See also H. Hilgenkamp, J. Mannhart, B. Mayer, Ch. Gerber, J. R. Kirtley, K. A. Moler, and M. Sigrist, in *Proceedings of International Symposium ASM-CCD*, September 1996 (Bombay, India), edited by R. Pinto *et al.* (Wiley Eastern, New Delhi, in press). For another class of tunneling spectroscopy involving various types of junctions of metal, insulator, *d*-wave superconductor leading to the appearance of zero-bias conductance peaks which are strongly dependent on the angle of tunneling direction and crystal axes, see the following theoretical papers; S. Kashiwaya, Y. Tanaka, M. Koyanagi, H. Takashima, and K. Kajimura, Phys. Rev. B **51**, 1350 (1995); Y. Tanaka and S. Kashiwaya, Phys. Rev. Lett. **74**, 3451 (1995); S. Kashiwaya, Y. Tanaka, M. Koyanagi, and K. Kajimura, Phys. Rev. B **53**, 2667 (1996); Y. Tanaka and S. Kashiwaya, *ibid*. **53**, 9371 (1996); Another class of interesting theoretical work exhibiting strong anisotropy due to possible *d*-wave and *s*-wave structures in the Josephson effect in the *d*-wave/insulator/*d*-wave junction is by Y. Tanaka and S. Kashiwara, Phys. Rev. B **53**, R11957 (1996) and in the *d*-wave/*s*-wave junction by Y. Tanaka, Phys. Rev. Lett. **72**, 3871 (1994).

[2] P. Chaudhari and S. Y. Lin, Phys. Rev. Lett. **72**, 1084 (1994); A. G. Sun, D. A. Gajewski, M. B. Maple, and R. C. Dynes, *ibid*. **72**, 2267 (1994); C. M. Varma, J. Phys. Chem. Solids **56**, 1685 (1995); G. Deutscher, in *Proceedings of International Symposium ASMCCD* (Ref. 1).

[3] See, e.g., D. J. Scalapino, Phys. Rep. **250**, 329 (1995); K. Maki and M. T. Beal-Monod, Phys. Lett. A **208**, 365 (1995); P. A. Lee and K. Kuboki, J. Phys. Chem. Solids **56**, 1633 (1995); M. Sigrist and K. Ueda, Rev. Mod. Phys. **63**, 239 (1991).

[4] D. Pines, Physica C **185**, 120 (1991); D. Pines and P. Monthoux, J. Phys. Chem. Solids **56**, 1651 (1995).

[5] S. S. Jha, Ind. J. Pure Appl. Phys. **30**, 482 (1992).

[6] S. S. Jha, Pramana, J. Phys. **29**, L615 (1987); J. M. Wheatly, T. C. Hsu, and P. W. Anderson, Nature (London) **333**, 121 (1988).

[7] A. K. Rajagopal and S. S. Jha, Phys. Rev. B **47**, 2780 (1993), to be referred to as I; See also, Physica C **174**, 161 (1991), to be referred to as II.

[8] S. S. Jha and A. K. Rajagopal, Physica C **168**, 173 (1990); A. K. Rajagopal and S. S. Jha, Solid State Commun. **73**, 763 (1990).

[9] L. N. Bulaevskii and M. V. Zyskin, Phys. Rev. B **42**, 10 230

(1990); R. A. Klemm and S. H. Liu, *ibid*. **44**, 7526 (1991).
[10] A. K. Rajagopal and S. S. Jha, Phys. Rev. B **54**, 4331 (1996); A preliminary account of the extension of this work was presented in *Proceedings of International Symposium ASMCCD* (Ref. 1).
[11] O. V. Kovalev, *Irreducible Representations of the Space Groups* (Gordon and Breach, New York, 1965).
[12] See *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (NBS, Washington, DC, 1968).
[13] See, e.g., J. Kane and K. W. Ng, Phys. Rev. B **53**, 2819 (1996).
[14] R. Kleiner and P. Müller, Phys. Rev. B **49**, 1327 (1994); **50**, 3942 (1994). See also, P. Müller, in *Proceedings of International Symposium ASMCCD* (Ref. 1).