

ANK/MSD/CP-78012 Conf-940121--2

INTRA-VERSUS INTERLAYER PAIRING IN THE COPPER OXIDE SUPERCONDUCTORS: RESPONSE TO A MAGNETIC FIELD*

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Submitted to SPIE Conference on Superconducting Superlattices and Multilayers, Los Angeles, CA, January 23-28, 1994.

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^{*} Work Supported by the U.S. Department of Energy, BES-Materials Sciences, under Contract #W-31-109-ENG-38.

Intra-versus interlayer pairing in the copper oxide superconductors: Response to a magnetic field

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ABSTRACT

We have investigated the response of layered superconductors to an external magnetic field using the semiclassical phase approximation. The linearized gap equations have been derived, and solved numerically to calculate the upper critical field $H_{c2}(T)$ for layered superconductors with one or two layers per unit cell for both *s*-wave and interlayer BCS-like pairing mechanisms. In the weak-hopping limit the equations reduce to the Lawrence-Doniach form, and for general hopping the appropriate gap equations are derived and numerically analyzed. One encounters the familiar dimensional crossover in the $H_{c2,||}(T)$ curve for weak hopping. A different type of dimensional crossover can occur in the two-layer case with unequal intralayer or interlayer coupling strengths, such that at the dimensional crossover temperature, the magnetic field suppresses the superconductivity in the weakly coupled layers while leaving the strongly coupled layers superconducting. The effect is enhanced by unequal hopping strengths. The flux lattice consists of alternating superconducting and normal layers.

1. INTRODUCTION

Recently, we have examined the competing roles of intralayer and interlayer pairing interactions in layered superconductors with $1 \le N \le 4$, where N is the number of conducting layers per unit cell c-axis edge $s.^{1-5}$ In these papers, the intralayer pairing was assumed to have the s-wave, BCS form for quasiparticle pairing at local sites within a conducting layer, and the interlayer pairing interaction involved pairing between quasiparticles directly above and below one another on adjacent layers. In all cases, the c-axis conduction was assumed for simplicity to be coherent, as pictured for N = 2 in Fig. 1, and the magnetic field was absent. We investigated the superconducting gap anisotropy arising from such models, and found that it could depend upon the wavevector k_z normal to the layers, but was independent of the wavevector components k_x and k_y parallel to the layers. Hence, the questions of gap anisotropy and of the competition of order parameters (OPs) reduced to a solvable, one-dimensional problem, with gap functions periodic in $k_z s$.

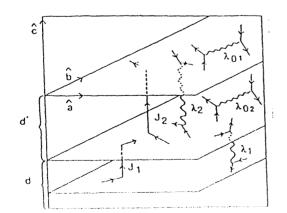


Fig. 1. Cross-sectional view of a N = 2 crystal section. The quasiparticles hop with matrix elements J_1 and J_2 between neighboring layers separated by d and d' = s - d, respectively. The intra- and interlayer pairing interactions $\lambda_{01}, \lambda_{02}, \lambda_1$, and λ_2 are also pictured.

For the one-layer case (N = 1), intralayer s-wave pairing gives rise to an isotropic, scalar singlet OP and energy gap, the amplitude of which which has a BCS temperature dependence below the transition temperature T_c . On the other hand, interlayer pairing stabilizes both a scalar singlet OP and a vector triplet OP, with associated gap functions proportional to $\cos k_z s$ and $\sin k_z s$, respectively, which depend strongly upon k_z , exhibiting nodes. These two OPs have identical T_c values, resulting in their coexistence in the superconducting state. The energy gap arising from interlayer pairing is also isotropic, however, as the free energy is a minimum when the amplitudes and phases of the singlet and the vector triplet components are all equal. When both intralayer and interlayer pairing interactions are present, the interaction leading to the higher bare T_c value completely suppresses the transition temperature of the other to zero, leading to an overall isotropic energy gap and a complete incompatibility of intralayer and interlayer pairing.

For multiple layers per unit cell, the competition between intralayer and interlayer pairing is more complex. In an N-layer system, interlayer coherent hopping results in N normal state quasiparticle bands. Since either the intralayer or interlayer pairing interactions are defined in real space (i. e., on or between the discrete layers), in momentum space they result in both intraband and interband pairing. Quasiparticles which form pairs within the same band can form a time-reversal invariant state, which is not suppressed by band parameters, such as interlayer hopping. On the other hand, interband pairing breaks time-reversal invariance, and the transition temperature is suppressed by interlayer hopping. In our previous analyses of the problem, we considered only the intraband pairing parts of the intra- and interlayer interactions. For N = 2, intralayer s-wave pairing results in isotropic gaps on both bands, even for inequivalent pairing strengths on the layers within the unit cell.¹⁻⁴ For $N \geq 3$ inequivalent s-wave intralayer pairing strengths give rise to gap functions which are different on each of the N bands, and weakly k_z -dependent.⁵ For this case, the quasiparticle density-of-states (DOS) curves exhibit non-monotonic structure inside the main peaks. For interlayer pairing with $N \geq 2$, one of the singlet state has the highest T_c , and its gap function dominates the behavior near to T_c . For N = 2, the dominant singlet gap function can be either nodeless, or have a pair of line nodes at fixed values $\pm k_{20}$ of k_z . When the singlet gap function is nodeless, the other singlet gap function and the triplet gap functions can all be neglected. On the other hand, when the singlet gap function has a pair of line nodes, the set of three triplet states with the higher bare T_c value can become non-vanishing at a second transition temperature, below the T_c of the dominant singlet state. For $N \geq 3$, the triplet states are usually negligible, but for N odd, the dominant singlet gap function always has a line node at $k_z = 0$, leading to an overall DOS which increases linearly with quasiparticle energy from zero at the Fermi energy E_F , and exhibits structure within the main DOS peaks. Such structure may have been observed in the cuprate superconductors $YBa_2Cu_3O_{7-\delta}$ (YBCO) and $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO).^{6,7}

Similar models have been treated in the usual mean-field approximation in real space by Tachiki et al.⁸ and by Bulaevskii and Zyskin⁹. In this approximation, the OPs are indexed according to the indexation of the discrete layers, corresponding to the interaction under consideration. For N = 1, there is no difference between the real space and the band representations, as there is only one quasiparticle band. For N = 2, however, the real space representation results in a higher T_c value than does the intraband projection of the momentum-space representation, at least for weak interlayer hopping. For strong interlayer hopping, there is no difference between the real space and intraband representations, as interband pairing is suppressed.¹⁰

Recently, we have extended our investigations of intralayer and interlayer pairing in the N = 1, 2 systems to include an external magnetic field in an arbitrary direction.¹¹ By use of the semiclassical phase approximation, the magnetic vector potential can be incorporated into the problem through an external wave vector. We have calculated the linearized gap equation, including the Pauli paramagnetism present for antiparallel-spin pairing states. In each case, we have derived the effective linearized Lawrence-Doniach gap equation, which can be used to calculate the upper critical field H_{c2} for an arbitrary field direction. In all cases, the quasiparticle pairs obey a Schrödinger equation with a generalized Lawrence-Doniach potential, containing an harmonic potential arising from the component of the magnetic field normal to the layers, and a periodic part arising from the component of the magnetic field parallel to the layers. This periodic potential is responsible for dimensional crossover effects for the field parallel to the layers at T^* , below which the vortex cores fit between the superconducting layers. For N = 2, the behavior near to T_c for intralayer and interlayer pairing is essentially indistinguishable. With different intralayer or interlayer pairing strengths, however, the details of the dimensional crossover are altered from those of equal intra- or interlayer pairing, as the order parameter corresponding to the weaker of the two interactions is suppressed relaive to that corresponding to the stronger interactions. Hence, the vortex cores can penetrate the weakly-paired layers

as well as the interstitials, leaving the strongly-paired layers superconducting. In other words, the lattice parameter characterizing dimensional crossover is the *c*-axis unit cell edge *s*. For N = 1, however, interlayer pairing favors triplet pairing¹², except for the field near to parallel to the layers in the vicinity of T_c . Hence, the parallel-field configuration can exhibit an interesting singlet-triplet transition.¹¹

2. THE ONE-LAYER MODELS

2.1 Intralayer BCS pairing

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We assume there is one conducting layer per unit cell which is infinitely thin. The layers are separated by a distance s, which also comprises the c-axis unit cell edge. We use units in which $\hbar = c = k_B = 1$. In the presence of an external magnetic field \vec{H} , there is a local magnetic induction $\vec{b} \cdot (\mathbf{r}, z) = \vec{\nabla} \times \vec{A} \cdot (\mathbf{r}, z)$, where $\vec{b} = (\mathbf{b}, b_z)$ and $\vec{A} = (\mathbf{A}, A_z)$, and bold-faced quantities are two-dimensional vectors, such as $\mathbf{A} = (A_x, A_y)$. The single quasiparticle part H_0 of the Hamiltonian $H = H_0 + V$ is taken to have the gauge-invariant form

$$H_{0} = \sum_{j\sigma} s \int d^{2}\mathbf{r} \psi_{j\sigma}^{\dagger}(\mathbf{r}) \xi_{0\sigma}(\mathbf{r}) \psi_{j\sigma}(\mathbf{r}) + J \sum_{j\sigma} \left[s \int d^{2}\mathbf{r} \psi_{j-1,\sigma}^{\dagger}(\mathbf{r}) \psi_{j\sigma}(\mathbf{r}) \exp[i\phi_{j}(\mathbf{r})] + H.c. \right], \quad (1a)$$

where $\psi_{j\sigma}(\mathbf{r})$ annihilates a quasiparticle with spin $\sigma = \pm$ at position \mathbf{r} in the j^{th} layer, J is the quasiparticle hopping integral between adjacent layers,

$$\xi_{0\sigma}(\mathbf{r}) = [-i\nabla - e\mathbf{A}(\mathbf{r})]^2 / 2m_0 - E_F - \sigma I, \qquad (1b)$$

where e is the quasiparticle charge, m_0 is the bare effective mass for free quasiparticle motion parallel to the layers, $I = g\mu_B/2$ is one-half of the Zeeman energy splitting, and we have assumed $\mathbf{A}(\mathbf{r})$ independent of the layer index near to H_{c2} . The phase factor in Eq. (1a) is given by $\phi_j(\mathbf{r}) = esA_z(\mathbf{r})$, assuming A_z independent of z near H_{c2} , and the s-wave intralayer pairing interaction V has the form

$$V = -\frac{1}{2}\lambda_0 \sum_{j\sigma} s \int d^2 \mathbf{r} \psi_{j\sigma}^{\dagger}(\mathbf{r}) \psi_{j,-\sigma}^{\dagger}(\mathbf{r}) \psi_{j,-\sigma}(\mathbf{r}) \psi_{j\sigma}(\mathbf{r}).$$
(1c)

Such a model could be obtained from Fig. 1 by setting $J_1 = J_2 = J$, $\lambda_{01} = \lambda_{02} = \lambda_0$, and $\lambda_1 = \lambda_2 = 0$, d = d' = s/2, and then letting $s \to 2s$.

In this treatment, we assume $H \approx H_{c2}$, so that $\overrightarrow{b} = \overrightarrow{H}$ can be taken to be a constant. The temperature Green's function matrix in constructed in the usual way,

$$G_{jj'}^{\alpha\beta}(\mathbf{r},\mathbf{r}',\tau-\tau') \equiv -\langle T[\psi_{j\alpha}(\mathbf{r},\tau)\psi_{j'\beta}^{\dagger}(\mathbf{r}',\tau')]\rangle, \qquad (2a)$$

$$F_{jj'}^{\alpha\beta}(\mathbf{r},\mathbf{r}',\tau-\tau') \equiv \langle T[\psi_{j\alpha}(\mathbf{r},\tau)\psi_{j'\beta}(\mathbf{r}',\tau')] \rangle, \qquad (2b)$$

and similarly for the G^{\dagger} and F^{\dagger} functions, where $\psi_{j\sigma}(\mathbf{r},\tau)$ is the quasiparticle annihilation operator at temperature τ in the Heisenberg representation. The gap function $\Delta_j(\mathbf{r})$ is given by

$$\Delta_0(\mathbf{r}) = -T \sum_{|\omega| \le \omega_{||}} \lambda_0 F_{jj}^{\sigma, -\sigma}(\mathbf{r}, \mathbf{r}, \omega), \qquad (3)$$

is taken to be independent of j, and the sum over the Matsubara frequencies ω is cut off at ω_{\parallel} . We assume that the semiclassical approximation for the magnetic field dependence of the Green's function in the form appropriate for a layered superconductor.¹³⁻¹⁶ The inverse of the Fourier transform of $G_{jj'}^{0\sigma}(\mathbf{r} - \mathbf{r}', \omega)$ is given by

$$G^{0\sigma^{-1}}(k,\omega) = i\omega - \xi_{0\sigma}(\mathbf{k}) - 2J\cos k_z s, \qquad (4)$$

where $k \equiv (\mathbf{k}, k_z)$ and $\xi_{0\sigma}(\mathbf{k}) = \mathbf{k}^2/2m_0 - E_F - \sigma I$ is the Fourier transform of Eq. (1b) in the absence of the vector potential. The expression for the linearized gap function is readily found to be,

$$\Delta_0(\mathbf{r}) = T \sum_{|\omega| \le \omega_0} \sum_{k'} \lambda_0 G^{0+}(k'_+, \omega) G^{0-}(-k'_-, -\omega) \Delta_0(\mathbf{r}), \tag{5a}$$

$$k'_{\pm} = (\mathbf{k}' \pm \mathbf{q}/2, k'_{z} \pm q_{z}/2),$$
 (5b)

$$\mathbf{q} = \mathbf{\Pi}(\mathbf{r}) \equiv -i\nabla - 2e\mathbf{A}(\mathbf{r}),\tag{5c}$$

$$q_z(\mathbf{r}) = -2eA_z(\mathbf{r}). \tag{5d}$$

Hence, the magnetic vector potential is incorporated into the problem by use of the external wavevector $\vec{q} = (q, q_z)$. In Eq. (5c) $\Pi(\mathbf{r})$ is the two-dimensional canonical momentum operator.

The k' integration is readily performed, leading to

$$\left(\frac{1}{4m_0}\Pi^2(\mathbf{r}) + g_0(q_z \ I)\right)\Delta_0(\mathbf{r}) = \frac{1}{b_0 E_F}\ln(T_c/T)\Delta_0(\mathbf{r}),\tag{6a}$$

$$1 = \lambda_0 N(0) a_{||}(T_c), \tag{6b}$$

$$a_{\parallel,\perp}(T) = \ln(2\gamma\omega_{\parallel,\perp}/\pi T), \tag{6c}$$

 $b_0(T) = 7\zeta(3)/[8(\pi T)^2]$, $N(0) = m/(2\pi s)$ is the band density of states at the Fermi level, $\gamma = 1.781$, and $g_0(q_z, I)$ is a periodic function¹¹ of $q_z s$ with period 2π . The transition temperature T_c is given by Eq. (61). For small J/E_F and I/E_F , we may expand Eq. (6a), yielding

$$\left(\frac{1}{4m_0}\Pi^2(\mathbf{r}) + \frac{J^2}{E_F}[1 - \cos(2eA_z s)]\right)\Delta_0(\mathbf{r}) = \frac{1}{b_0 E_F} \left(\ln(T_c/T) - 2b_0 I^2\right)\Delta_0(\mathbf{r}),\tag{7}$$

where $\Pi(\mathbf{r})$ is given by Eq. (5c). Equation (7) has the form of the linearized order parameter equation in the Lawrence-Doniach phenomenological model of a layered superconductor¹⁷ for an arbitrary field direction.^{14,18} The effective mass for propagation along the *c*-axis in the superconducting state is obtained by expanding Eq. (7) for small q_z , which for small J reduces to $M = E_F/2J^2s^2$.

Numerical calculations¹¹ with the full $g_0(q_z, I)$ have been performed for the field parallel to the layers, choosing $\vec{b} = (H, 0, 0)$ with $\vec{A} = (0, 0, Hy)$. In this case, Eq. (6a) reduces to the form of the Hill equation, a Schrödinger equation with a periodic potential. It is thus an eigenvalue equation, the lowest eigenvalue of which determines the upper critical field $H_{c2,||}$ parallel to the layers. In the weak hopping limit, Eq. (8) reduces to the Mathieu equation, as discussed previously¹⁴. For more general hopping strengths J, the eigenvalue equation may be solved numerically. To do so, we employ a variational technique, using the periodic trial solution with variational parameter α ,

$$\Delta_0(y) = C \exp[-\alpha q_z^2/2], \quad \text{for} \quad -\pi/s \le q_z \le \pi/s, \tag{8}$$

which is repeated outside the first zone. Note that $q_z = -2eHy$. Such a trial solution is a simplified version of that which has been successfully used in the study of $H_{c2,||}$ in superconducting superlattices.¹⁹ This form of the trial solution is exact in the low-field, three-dimensional (3D) limit very near to T_c and in the highfield, two-dimensional (2D) limit well below the dimensional crossover temperature T^* . However, it is only qualitative in the vicinity of T^* given in the Lawrence-Doniach model by $\xi_{\perp}(T^*) = s/\sqrt{2}$, where $\xi_{\perp}(T)$ is the Ginzburg-Landau coherence length normal to the layers.

In Fig. 2, $H_{c2,II}(T)/H_0$ is shown for this N = 1 intralayer pairing model, for various values of J/T_c , where $H_0 = m_0 T_c/k_F s[c]$. The solid curves are the results obtained from the orbital pairbreaking alone, obtained by setting I = 0, and the dashed curves include both orbital and Pauli pairbreaking. Dimensional crossover is exhibited by the strong upward curvature of $H_{c2,II}(T)$ for the weak hopping curves $(J/T_c = 0.5)$.

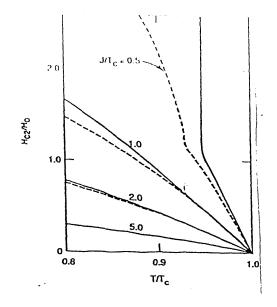


Fig. 2. The upper critical field $H_{c2,||}(T)$ relative to H_0 is plotted versus T/T_c for the onelayer model with intralayer s-wave pairing, are plotted for different values of J/T_c , and $H_0 = m_0 T_c/k_F s|e|$. Solid curves are the result of orbital pairbreaking alone (I = 0), and dashed curves include both orbital and Pauli pairbreaking effects, assuming $g/2k_F s = 0.2$.

2.2 Interlayer pairing

For interlayer pairing with N = 1, we assume H_0 is again given by Eq. (1a), but the pairing interaction V is given by

$$V = -\frac{1}{2}\lambda_1 \sum_{j\sigma\sigma'} s \int d^2 \mathbf{r} \psi_{j\sigma}^{\dagger}(\mathbf{r}) \psi_{j+1,\sigma'}^{\dagger}(\mathbf{r}) \psi_{j+1,\sigma'}(\mathbf{r}) \psi_{j\sigma}(\mathbf{r}), \qquad (9)$$

where all values of $\sigma, \sigma' = \pm$ are allowed, since the interaction is assumed to be spin-independent, and the Pauli exclusion principle does not apply to pairing between quaiparticles at different positions. This model is also illustrated in Fig. 1, with $J_1 = J_2 = J$, $\lambda_{01} = \lambda_{02} = 0$, $\lambda_1 = \lambda_2$, d = d' = s, and letting $s \to 2s$. Hence, both singlet and triplet paring states are allowed, and they have identical transition temperatures, even in the presence of spin-independent scattering, so they are essentially degenerate, and it is inappropriate to consider one without the other. As we shall see, the magnetic field breaks this degeneracy, but the manner in which the degeneracy is broken is rather complicated. We define the interlayer order parameters in a manner analogous to Eq. (3),

$$\Delta_{j,j\pm 1}^{\sigma\sigma'}(\mathbf{r}) = -T \sum_{|\omega| \le \omega_{\perp}} \lambda_1 F_{j,j\pm 1}^{\sigma\sigma'}(\mathbf{r},\mathbf{r},\omega).$$
(10)

We then Fourier transformation in the sum of and difference between the layer indices with wavevectors k'_z and k_z , respectively. At H_{c2} , we may neglect the k'_z dependence of the gap functions, as such dependence arises from the center-of-mass motion of the pairs, and is only important if one considers fluctuation effects. The resulting gap function equation is then

$$\Delta^{\sigma\sigma'}(k_z,\mathbf{r}) = T \sum_{|\omega| \le \omega_{\perp}} \sum_{k'} \lambda_1 \cos[(k_z - k'_z)s] G^{0\sigma}(k'_+,\omega) \Delta^{\sigma\sigma'}(k'_z,\mathbf{r}) G^{0\sigma'}(-k'_-,-\omega), \tag{11}$$

where the k'_{\pm} are given by Eqs. (5b)-(5d). As shown previously¹, for the uniform, field-indepedent situation, the gap functions can be written as $\Delta_s(k_z, \mathbf{r}) = \sqrt{2} \cos(k_z s) \Delta_s(\mathbf{r})$ and $\Delta_{tm}(k_z, \mathbf{r}) = \sqrt{2} \sin(k_z s) \Delta_{tm}$, where $m = 0, \pm 1$ are the triplet spin states. In zero field, the three triplet spin states are all degenerate with with singlet state. In a magnetic field, this degeneracy is broken. The linearized gap function equations are found to be

$$\left(\frac{1}{4m_0}\Pi^2(\mathbf{r}) + g_s(q_z, I)\right)\Delta_s(\mathbf{r}) = \frac{1}{2b_0E_F}\ln(T_c/T)\Delta_s(\mathbf{r}),$$
(12a)

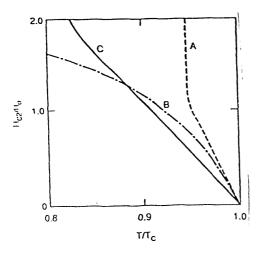
$$\left(\frac{1}{4m_0}\Pi^2(\mathbf{r}) + g_t(q_z, I)\right)\Delta_{t0}(\mathbf{r}) = \frac{1}{2b_0E_F}\ln(T_c/T)\Delta_{t0}(\mathbf{r}), \tag{12b}$$

$$\left(\frac{1}{4m_0}\mathbf{\Pi}^2(\mathbf{r}) + g_t(q_z, 0)\right)\Delta_{t\pm}(\mathbf{r}) = \frac{1}{2b_0E_F}\ln(T_{c\pm}/T)\Delta_{t\pm}(\mathbf{r}).$$
(12c)

where the transition temperatures T_c and $T_{c\pm}$ are given by $1 = \frac{1}{2}\lambda_1 N(0)a_{\perp}(T_c)$ and $1 = \frac{1}{2}\lambda_1 N_{\pm}(0)a_{\perp}(T_{c\pm})$, where $a_{\perp}(T)$ is given by Eq. (6b), $N_{\pm}(0) \approx N(0) \pm 1N'(0)$ are the single quasiparticle densities of states for the up (+) and down (-) spins, and N'(0) is the derivative of the density of states at the Fermi level. In Eq. (12), $g_s(q_z, I)$ and $g_t(q_z, I)$ are slightly different periodic functions of $q_z s$ with period 2π , the sum of which would equal $g_0(q_z, I)$ if $\omega_{\perp} = \omega_{\parallel}$.

In a field, since $N_{\pm}(0)$ differs form N(0) by an amount linear in the field, the T_c values for the three triplet states are split, with one of the parallel-spin states having the highest T_c value overall. Note that both parallel-spin states do not exhibit Pauli pairbreaking, buth that both the singlet and the antiparallelspin triplet states do exhibit Pauli pairbreaking. In addition, since $g_s(q_z, I)$ is different from $g_t(q_z, I)$, the amounts of prbital pairbreaking present in the singlet and triplet states is different. Expanding for small J and I, we obtain $g_s(q_z, I) \approx (J^2/2E_F)[1 - \cos q_z s] + I^2/E_F$, and $g_t(q_z, I) \approx (3J^2/2E_F)[1 - \cos q_z s] + I^2/E_F$. Thus, in the weak-hopping limit, the effective masses for propagation along the c-axis direction are $M_s = E_F/J^2s^2$ and $M_t = E_F/3J^2s^2$, respectively. As for the N = 1 intralayer pairing case, we have performed a numerical evaluation of $H_{c2,||}(T)$ for the interalyer pairing singlet and triplet states, using the same variational procedure [Eq. (8)].

For $\overline{H}||\hat{c}$, the orbital effects on all of the OPs are the same, so the Pauli pairbreaking determines the relative importance of the states, which would be otherwise degenerate. Depending upon the sign of IN'(0), one of the parallel-spin states will have the highest T_c , either T_{c+} or T_{c-} . For the purposes of discussion, we let this state be the Δ_{t+} state with transition temperature T_{ct} . Just below T_{c+} , only Δ_{t+} with be non-vanishing. However, at the temperature $T_{cs} < T_{ct}$, the system undergoes a second second-order phase transition to the ST state¹, in which Δ_s and the other parallel-spin state Δ_{t-} are also non-vanishing. In the parallel-spin state $T_{cs} < T < T_{ct}$, the gap function will have line nodes at $k_z = 0, \pm \pi/s$. Below T_{cs} , the non-vanishing Δ_s removes the nodes, leading to a gap function which is nearly is tropic at low temperature, the only anisotropy arising from the Pauli pairbreaking terms. Such behavior was first discussed by Efetov and Larkin,¹² and details of the argument are given in Ref. (11).



5.2

Fig. 3. Curves of $H_{c2,||}(T)/H_0$ versus T/T_c for the N = 1 interlayer-pairing states, including Pauli corrections. Curve A is for the singlet state neglecting Pauli pairbreaking. Curve B is for the singlet state, including Pauli pairbreaking effects with $g/2k_Fs = 1$. Curve C is for the parallel-spin triplet state of the same model. The system undergoes a first-order phase transition at the point where curves B and C cross.

For $\overline{H} \perp \hat{c}$, the situation is more interesting. In the low field limit, both the Pauli correction to N(0)and the orbital correction are linear in the field strength, but the orbital correction is generally much more important, obeying $|Jev_F|s/T_c^2 >> \mu_B|N'(0)|/N(0)$, where v_F is the Fermi velocity parallel to the layers. In this case, we can set $T_{c\pm} = T_c$, at least for a qualitative discussion. Since the interlayer pair hopping costs more energy for the triplet states, the *singlet* state Δ_s is favored near to T_c . At low temperatures, dimensional crossover removes the orbital paribreaking for both singlet and triplet states, so the Pauli pairbreaking dominates. This leads to a crossover from the singlet state Δ_s just below T_c to the lower-energy parallel-spin triplet state Δ_{t+} at a lower temperature, with a corresponding first-order phase transition. This behavior is pictured in Fig. 3. With regard to nodes in the gap function, we note that just below T_c , the singlet gap function proportional to $\cos k_2 s$ prevails. This function has line nodes at $k_2 = \pm \pi/2s$. While we have not investigated the competition between the various states in a magnetic field parallel to the layers, it seems likely that the two parallel-spin states could combine with the singlet state (as for $\mathbf{H}[c]$) to remove the nodes at lower temperature, provided that the temperature at which this occurred was above the first-order transition to the purely parallel-spin triplet state. It remains to be seen if the singlet state could recombine with the parallel-spin triplet states at a temperature lower than this first-order transition.

3. THE TWO-LAYER MODELS

3.1. Intralayer BCS pairing

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The single quasiparticle Hamiltonian for a superconductor with two layers per unit cell c-axis edge is taken to be of the form

$$H_{0} = \sum_{j\sigma} s \int d^{2}\mathbf{r} \left[\frac{1}{2} \sum_{n} \psi_{jn\sigma}^{\dagger}(\mathbf{r}) \xi_{0\sigma}(\mathbf{r}) \psi_{jn\sigma}(\mathbf{r}) + J_{1} \psi_{j1\sigma}^{\dagger} \psi_{j2\sigma} e^{i\phi_{j1}(\mathbf{r})} + J_{2} \psi_{j-1,2\sigma}^{\dagger} \psi_{j1\sigma} e^{i\phi_{j2}(\mathbf{r})} + H.c. \right], \quad (13)$$

where $n = 1, 2, J_1$ and J_2 are the interlayer hopping matrix elements pictured in Fig. 1, $\xi_{0\sigma}(\mathbf{r})$ is given by Eq. (1b), the interlayer spacings are d within a unit cell and d' = s - d between neighboring unit cells, respectively, $\phi_{j1}(\mathbf{r}) = edA_z(\mathbf{r})$, and $\phi_{j2}(\mathbf{r}) = ed'A_z(\mathbf{r})$ are required for gauge invariance near to H_{c2} . In the absence of the pairing interaction, H_0 can be diagonalized by the canonical transformation.¹⁻⁴ giving rise to two normal-state quasiparticle bands indexed by \pm . As for the N = 1 case, we employ the quasiclassical approximation to write the Green's function in the presence of a magnetic field in terms of the bare Green's function in the absence of the vector potential,

$$G_{\pm}^{0\sigma^{-1}}(k,\omega) = i\omega - \xi_{0\sigma}(\mathbf{k}) \mp \epsilon_{\perp}(k_z), \qquad (14)$$

where $\xi_{0\sigma}(\mathbf{k})$ is the same as in Eq. (4), and $\epsilon_{\perp}(k_z) = [J_1^2 + J_2^2 + eJ_1J_2 \cos k_z s]^{1/2}$.

For BCS intralayer pairing with N = 2, the pairing interaction may be written as

$$V = -\frac{1}{2} \sum_{jn\sigma} \lambda_{0n} s \int d^2 \mathbf{r} \psi_{jn\sigma}^{\dagger}(\mathbf{r}) \psi_{jn,-\sigma}^{\dagger}(\mathbf{r}) \psi_{jn,-\sigma}(\mathbf{r}) \psi_{jn\sigma}(\mathbf{r}), \qquad (15)$$

which is pictured in Fig. 1. Although it is possible to treat the case of inequivalent conducting layers with inequivalent two-dimensional band structures^{10,20}, we assume for simplicity that the layers have the same zero-field two-dimensional band structures $\xi_{0\sigma}(\mathbf{k})$, but allow for inequivalent intralayer pairing interactions λ_{01} and λ_{02} . As a result, each layer within a unit cell has its own gap function $\Delta_n(\mathbf{r})$, obtained from

$$\Delta_{n}(\mathbf{r}) = T \sum_{|\omega| \le \omega_{||}} \lambda_{0n} \sum_{k'm} G_{nm}^{0\sigma}(k'_{+}, \omega) G_{mn}^{0, -\sigma}(-k'_{-}, -\omega) \Delta_{m}(\mathbf{r}), \tag{16}$$

where n, m = 1, 2 index the layers within a unit cell, and the k'_{\pm} are given by Eqs. (5b)-(5d).

Although in the N = 1 case, intralayer pairing gives rise to an expression for T_c [Eq. (6b)] which is independent of the hopping J, for the general two-layer problem with inequivalent intralayer pairing interactions, T_c depends upon the hopping matrix elements J_1 and J_2 . Hence, we must first determine the expression for the zero-field T_c , before we can write down the equations for the gap functions in the presence of a magnetic field. For simplicity, in the following we shall ignore the Pauli limiting, but such effects always occur for singlet states, as for the N = 1 cases discussed in §2. In the absence of a magnetic vector potential, the linearized gap equations may be written as

$$\Delta_n = \lambda_{0n} N(0) \sum_{n'} [a_{||}(T) \delta_{nn'} - (-1)^{n-n'} \delta a(T)] \Delta_{n'}, \qquad (17)$$

where $\delta a(T)$ gives rise to pairbreaking due to the interlayer hopping. The critical temperature T_c is then found by setting the determinant of Eq. (19) equal to zero.

There are usually two solutions for T_c obtained from Eq. (17), and the physical solution is the higher T_c value. In the limit of no hopping $(J_1, J_2 \rightarrow 0)$, $\delta a(T) \rightarrow 0$, so Eq. (17) factorizes. The critical temperature T_{c0} , obtained in this limit of no interlayer hopping, is then

$$\lambda_{\mathbb{N}} N(0) a_{\mathrm{H}}(T_{c0}) = 1, \tag{18a}$$

where $\lambda_{>}$ is the larger of $\lambda_{01}, \lambda_{02}$. For small $J_1, J_2, \delta a(T) \approx b_0(J_1^2 + J_2^2)/2$, which is pairbreaking, decreasing T_c from its bare value T_{c0} . In the opposite limit of strong interlayer hopping, $\max(J_1, J_2) >> \omega_{\parallel}, \delta a(T) \approx \frac{1}{2}a_{\parallel}(T)$, and T_c is given by

$$\overline{\lambda}N(0)a_{\rm H}(T_c) = 1, \tag{18b}$$

where $\overline{\lambda} = (\lambda_{01} + \lambda_{02})/2$ is the average of the intralayer pairing interactions. A plot of T_c/T_{c0} versus J_2/T_{c0} is presented by curve A in Fig. 4 for $J_1/J_2 = 0.8$, $\lambda_{02}/\lambda_{01} = 0.9$, and $N(0)\lambda_{01} = 0.5$. In the limits of weak and strong hopping, T_c/T_{c0} approaches unity and 0.9, respectively. Note that the strong hopping limit is obtained when only one of the interlayer hoppings is large, as well as when both of them are large.

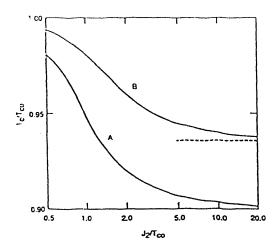


Fig. 4. Plots of T_c relative to the respective bare value T_{c0} obtained in the absence of interlayer hopping, as a function of J_2/T_{c0} , for two models with N = 2. Curve A is for intralayer pairing with $\lambda_{02}/\lambda_{01} = 0.9$, $J_1/J_2 = 0.8$, and $N(0)\lambda_{01} =$ 0.5. For very strong hopping, $T_c/T_{c0} \rightarrow 0.9$, the band limit. Curve B is for interlayer pairing with $\lambda_1/\lambda_2 = 0.9$, $J_1/J_2 = 0.7$, and $N(0)\lambda_2 = 0.5$.

We now consider a finite magnetic field. In order to simplify the equations as much as possible, we shall neglect the Pauli contributions, but these can be inserted in a manner entirely analogous to that for the N = 1 case. Expanding Eq. (16) for small q, and carrying out the k' integrations, we have the system of equations of the form

$$\sum_{n'} \left(\frac{1}{4m_0} \Pi^2(\mathbf{r}) t_{nn'}(q_z) + g_{nn'}(q_z) \right) \Delta_{n'}(\mathbf{r}) = \frac{1}{b_0 E_F} \left(a_{||}(T) - \frac{1}{\lambda_{0n} N(0)} \right) \Delta_n(\mathbf{r}), \tag{19}$$

where $t_{nn'}(q_z)$ and $g_{nn'}(q_z)$ are periodic functions¹¹ of $q_z s$ with period 2π . While these functions appear to also depend upon d as well as upon s, the d-dependence only enters the relative phases of the constituents of the resulting gap functions, but does not contribute to any measureable quantity.

In the weak hopping limit $J_1, J_2 \ll T_c$, the functions $t_{nn'}$ and $g_{nn'}$ may be evaluated analytically, and the 2×2 matrix diagonalized, leading to

$$\left(\frac{1}{4m_0}\Pi^2(\mathbf{r}) \pm \frac{1}{2E_F} [J_1^4 + J_2^4 + 2J_1^2 J_2^2 \cos q_z s]^{1/2}\right) \Delta_{\pm}(\mathbf{r}) = \frac{1}{b_0 E_F} \left(a_{||}(T) - \frac{1}{\lambda_{01} N(0)} - \frac{b_0}{2} (J_1^2 + J_2^2)\right) \Delta_{\pm}(\mathbf{r}), (20)$$

where the $\Delta_{\pm}(\mathbf{r})$ are the two linearly independet gap functions obtains in diagonalizing the matrix. Equation (20) was used by Lee, Klemm, and Johnston²¹ to fit the fluctuation diamagnetism data of YBa₂Cu₃O₇, and was derived phenomenologically.²² In terms of fluctuations, the quantity q_z is a variable of integration, and $\Pi^2 \rightarrow \mathbf{k}^2$ is another variable of integration. Note that there are two order parameter *bands*, with different T_c values. In this case, only the (-) band with the higher, unsuppressed T_c value [given by either Eq. (18a) or (18b)] is relevant for the study of H_{c2} . This band has a q_z dispersion which is similar to that of the Lawrence-Doniach model, and an effective mass for c-axis propagation given by $M = E_F(J_1^{-2} + J_2^{-2})/s^2$.

Another interesting limit is the case of two very different layers, $|\lambda_{01}| >> |\lambda_{02}|$, for which the superconductivity in the n = 2 layers is primarily obtained from the proximity of the more superconducting n = 1 layers. In this case, we may eliminate Δ_2 from Eq. (19) to obtain,

$$\left[\frac{1}{4m_0}\mathbf{H}^2(\mathbf{r}) - \frac{b_0\lambda_{01}N(0)[J_1^4 + J_2^4 + 2J_1^2J_2^2\cos q_{\mathbb{F}}\mathbf{s}]}{4E_F(\lambda_{01}/\lambda_{02} - 1)}\right]\Delta_1(\mathbf{r}) - \frac{1}{b_0E_F}\left[a_{||}(T) - \frac{1}{\lambda_{01}N(0)} - \frac{b_0}{2}(J_1^2 + J_2^2)\right]\Delta_1(\mathbf{r}).$$
(21)

In this case, there is a suppression of T_c due to interband pairbreaking, and a Lawrence-Doniach dispersion characterized by a *c*-axis effective mass given by $M = E_F(\lambda_{01}/\lambda_{02} - 1)/[b_0N(0)\lambda_{01}J_1^2J_2^2s^2]$.

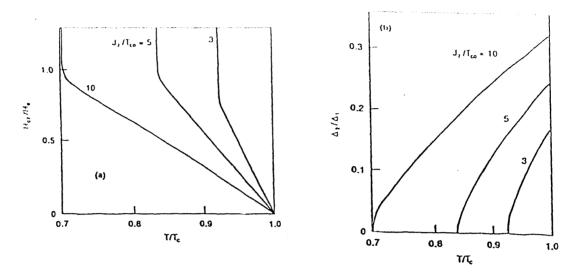


Fig. 5. (a) Shown are $H_{c2,||}(T)$ curves neglecting Pauli pairbreaking for an N = 2 intralayer pairing model with $\lambda_{02}/\lambda_{01} = 0.5$, $J_1/J_2 = 0.1$, and $\lambda_{01}N(0) = 0.5$. Dimensional crossover is possible for $J_1/T_c = 1$, which corresponds to rather large values of $J_2/T_c = 10$. (b) The magnitude $|\Delta_2/\Delta_1|$ of the ratio of the intralayer order parameters calculated at $H_{c2,||}(T)$ for the same parameters as in (a), as a function of T/T_c and hopping strength J_2/T_c . The curves demonstrate that at the dimensional crossover temperature T^* , the order parameter in layer 2 is suppressed.

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In numerical evaluation of $H_{c2,||}$, we have neglected the Pauli paribreaking, as it plays a similar role as in the N = 1 case. The orbital pairbreaking is a bit different than for N = 1, since there are two, inequivalent order parameters. Hence, we have used a variational procedure which is an extension of that used for the N = 1 case,

$$\Delta_n(q_z) = C_n \exp[-\alpha q_z^2/2], \text{ for } -\pi/s \le q_z \le \pi/s, \tag{22}$$

for n = 1, 2, where both α and C_2/C_1 are variational parameters. These variational forms are used to solve Eq. (19) with the full expressions for $t_{nn'}$ and $g_{nn'}$ given elsewhere¹¹. The ratio C_2/C_1 is chosen to diagonalize the equations, and α is then chosen so as to give the maximum $T_c(H)$. The resulting $H_{c2,||}(T)$ curves are shown in Fig.5 (a). All of these curves are linear near to T_c , as in the anisotropic Ginzburg-Landau model, but show dimensional crossover at the temperature T^* at which $H_{c2,||}(T)$ diverges in the absence of Pauli pairbreaking.

When one of the hoppings is much larger than the other one, the weak hopping determines the dimensional crossover. When $J_2/\omega_{||} >> 1$ and $J_1/\omega_{||} << 1$, the two layers within the unit cell are strongly coupled together, and act as a single layer which is weakly coupled to its neighboring layers. In this limit, the linearized gap equation reduces to that of Eq. (6), except that J is replaced with $J_1/2$ and λ_0 is replaced by the average interaction $\overline{\lambda} = (\lambda_{01} + \lambda_{02})/2$. In Fig. 5 (a), we have shown plots of $H_{c2,||}(T)/H_0$ versus T/T_c for $\lambda_{02}/\lambda_{01} = 0.5$, $N(0)\lambda_{01} = 0.5$, $J_1/J_2 = 0.1$, for various values of J_2/T_c . The sharp upward curvature at the dimensional crossover temperature T^* is expected to be smoothed somewhat by the inclusion of Pauli pairbreaking effects. These curves demonstrate that dimensional crossover occurs when the smaller hopping (in this case, $J_1 = 0.1J_2$) is less than or comparable to T_c . The calculations also showed that the mixing ratios of Δ_1 and Δ_2 is strongly affected by dimensional crossover. Below T^* , the order parameter corresponding to the layer with the weaker pairing interaction ceases to be superconducting, as shown in Fig. 5(b). This phenomenon is similar to that first discussed by Tachiki and Takahashi⁸ in superconducting superlattices, but is a bit different in that it does not depend upon the initial slope of $H_{c2,||}(T)$ as determined by the amount of impurity scattering, as their did effect. In our case, dimensional crossover occurs when the vortex cores extend over the entire unit cell edge s, not only over the insulating interstitial regions, but also suppressing the weakly superconducting layers. There is only one dimensional crossover temperature T^* in our N = 2 models.

3.2. Interlayer pairing

For the N = 2 interlayer pairing case, the interaction has the form

$$V = -\frac{1}{2} \sum_{j\sigma\sigma'} s \int d^2 \mathbf{r} \left(\lambda_1 \psi_{j1\sigma}^{\dagger}(\mathbf{r}) \psi_{j2\sigma'}^{\dagger}(\mathbf{r}) \psi_{j1\sigma}(\mathbf{r}) + \lambda_2 \psi_{j-1,2\sigma}^{\dagger}(\mathbf{r}) \psi_{j1\sigma'}^{\dagger}(\mathbf{r}) \psi_{j1\sigma'}(\mathbf{r}) \psi_{j1\sigma'}(\mathbf{r}) \psi_{j-1,2\sigma}(\mathbf{r}) \right).$$
(23)

The interactions λ_1 and λ_2 form pairs on adjacent layers in the same unit cell and in adjacent unit cells, respectively. After Fourier transformation over the unit cell indices, the gap equation in the semiclassical approximation becomes

$$\Delta_{nn'}^{\sigma\sigma'}(k_z,\mathbf{r}) = T \sum_{|\omega| \le \omega_{\perp}} \sum_{k'} V_{nn'}(k_z - k'_z) \sum_{mm'} G_{nm}^{0\sigma}(k'_{\perp},\omega) \Delta_{mm'}^{\sigma\sigma'}(k'_z,\mathbf{r}) G_{n'm'}^{0\sigma'}(-k'_{\perp},-\omega), \tag{24}$$

where k'_{\pm} are given by Eqs. (5b)-(5d), and it is understood that the operators in k'_{\pm} act to the left [upon $\Delta_{mm'}(k'_{z}, \mathbf{r})$]. The Fourier transform of the interlayer pairing interaction is an off-diagonal matrix of rank 2, with non-vanishing elements

$$V_{12}(k_z - k'_z) = \lambda_1 \exp[i(k_z - k'_z)d] + \lambda_2 \exp[-i(k_z - k'_z)d']$$
(25)

and $V_{21}(k_z - k'_z) = V_{12}^*(k_z - k'_z)$. Since it has been shown both in the weak hopping limit¹⁰ and in the strong hopping limit¹⁻⁴ that the highest T_c value for interlayer pairing with N = 2 occurs for one of the singlet states, we set $\sigma' = -\sigma$ and drop the spin indices on the gap functions. Thus, the only non-vanishing $\Delta_{nn'}$ are $\Delta_{12}(k_z,)$ and $\Delta_{21}(k_z, \mathbf{r})$. The structure of Eq. (28) leads to the useful parametrization,

$$\Delta_{12}(k_z, \mathbf{r}) = \overline{\Delta}_1(\mathbf{r}) \exp[ik_z d] + \overline{\Delta}_2(\mathbf{r}) \exp[-ik_z d'], \qquad (26)$$

and $\Delta_{21}(k_z, \mathbf{r})$ is obtained from Eq. (26) by changing the sign of k_z . Since d+d' = s, $\exp[ik_z d]$ and $\exp[-ik_z d']$ are mutually orthogonal functions over the full Brillouin zone, so that the gap equations may be separated into equations for the $\overline{\Delta}_n(\mathbf{r})$. After some algebra, we obtain

$$\sum_{n'} \left(\frac{1}{4m_0} \Pi^2(\mathbf{r}) \bar{t}_{nn'}(q_z) + \bar{g}_{nn'}(q_z) \right) \overline{\Delta}_{n'}(\mathbf{r}) = \frac{1}{b_0 E_F} \left(a_\perp(T) - \frac{1}{\lambda_n N(0)} \right) \overline{\Delta}_n(\mathbf{r}), \tag{27}$$

where the $\bar{t}_{nn'}$ and the $\bar{g}_{nn'}$ for n, n' = 1, 2 are periodic functions of $q_z s$ with period 2π , the detailed forms of which are given in Ref. (11). The transition temperature is obtained by setting $\Pi(\mathbf{r}) = 0$ and $q_z = 0$, and $T = T_c$, leading to a simple matrix of rank 2 which is easily diagonlized. In the absence of interlayer hopping, the bare transition temperature T_{c0} is given by Eq. (18a) with $\lambda_>$ in this case being the greater of λ_1 and λ_2 , repectively. A plot of T_c/T_{c0} versus J_2/T_{c0} is given in Fig. 4.

In the weak hopping limit $J_1, J_2 \ll T_c$, these functions may be expanded. Letting the renormalized coupling strengths be $\overline{\lambda}_1 = \lambda_1/[1 + \lambda_1 N(0)b_0 J_2^2]$ and $\overline{\lambda}_2 = \lambda_2/[1 + \lambda_2 N(0)b_0 J_1^2]$, for the special case $\overline{\lambda}_1 = \overline{\lambda}_2$, Eq. (28) reduces to

$$\left(\frac{1}{4m_0}\mathbf{\Pi}^2(\mathbf{r}) \pm \frac{J_1J_2}{E_F}(1-\cos q_2 s)\right)\overline{\Delta}_{\pm}(\mathbf{r}) = \frac{1}{b_0E_F}\left(a_{\pm}(T) - \frac{1}{\overline{\lambda}_1 N(0)} \pm b_0J_1J_2\right)\overline{\Delta}_{\pm}(\mathbf{r}),\tag{28}$$

where $\overline{\Delta}_4 = \overline{\Delta}_1 \pm \overline{\Delta}_2$. The order parameter $\overline{\Delta}_1$ has the higher T_c value, and for this state the *c*-axis effective mass is $M = E_F/2J_1J_2s^2$.

For general hopping and pairing strengths, the linearized equations for the order parameters in the presence of a magnetic field can be solved numerically to obtain the upper critical field $H_{c2,ll}(T)$. In Fig.

6(a), a set of $H_{c2,||}(T)/H_0$ versus T/T_c curves is shown for $\lambda_2/\lambda_1 = 0.5$, $J_1/J_2 = 0.2$, and $N(0)\lambda_1 = 0.5$, neglecting Pauli pairbreaking. Since dimensional crossover is determined by the weaker of the hopping strengths (J_1 in this case), it can occur for rather large values of the stronger hopping (J_2). In Fig. 6(b), we have plotted the ratio of the magnitudes of the order parameters $\overline{\Delta}_2$ and $\overline{\Delta}_1$ versus T/T_c , for the same parmaeters as in Fig. 6(a). Precisely as for the situation of inequivalent intralayer pairing with N = 2, the order parameter ($\overline{\Delta}_2$ in this case) corresponding to the weaker interlayer pairing interaction (λ_2) is suppressed below T^* . Hence, the magnetic response of a layered superconductor with N = 2 layers per unit cell cannot distinguish between intralayer and interlayer pairing, at least near to H_{c2} .

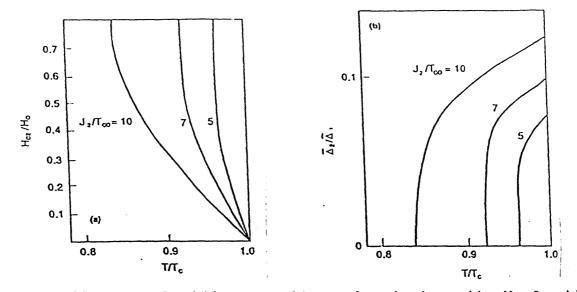


Fig. 6. (a) Shown are $H_{c2,||}(T)/H_0$ versus T/T_c curves for an interlayer pairing N = 2 model with $\lambda_2/\lambda 1 = 0.5$, $J_1/J_2 = 0.2$, and $\lambda_1 N(0) = 0.5$, for various values of J_2/T_{c0} . Dimensional crossover is possible for $J_1/T_{c0} \leq 2$, which occurs for rather large values of J_2/T_{c0} . (b) The ratio $|\overline{\Delta}_2/\overline{\Delta}_1|$ of the two interlayer pairing order parameters for N = 2, as a function of T/T_c for the same parameters as in (a). These curves demonstrate that at the dimensional crossover temperature T^* , the $\overline{\Delta}_2$ order parameter corresponding to the weaker pairing interaction λ_2 is suppressed.

4. SUMMARY AND DISCUSSION

We have derived the linearized gap function equations in the presence of a magnetic field for layered superconductors with one and two layers per unit cell, with either intralayer or interlayer BCS-like pairing interactions. In the limit of weak interlayer hopping, the equations reduce to the Lawrence-Doniach form, with c-axis dispersions proportional to $1 - \cos q_z s$ and pair hopping energies proportional to J_n^2/E_F . For more general hopping strengths, the equations for H_{c2} are similar to the Lawrence-Doniach form, with c-axis dispersions that are periodic functions of $q_z s$ with period 2π , but with more general mathematical forms.

For N = 1, $H_{c2,||}(T)$ can distinguish between intralayer BCS and interlayer BCS-like pairing interactions. While both situations exhibit the familiar dimensional crossover at T^* given by $\xi_{\perp}(T^*) = s/\sqrt{2}$, the interlayer pairing case can also exhibit a first order transition from the singlet state favored energetically near to T_c to the parallel-spin triplet state at lower temperatures. For the field parallel to the *c*-axis, interlayer pairing favors parallel-spin triplet pairing, whereas intralayer pairing favors singlet pairing. For N = 2, since singlet states are dominant for both intralayer and interlayer pairing, the H_{c2} measurements cannot distinguish between intralayer and interlayer pairing mechanisms. However, and interesting situation arises for either mechanism when one of the two pairing strengths is less than the other. In this case, below the dimensional crossover temperature T^* at which $H_{c2,||}(T)$ would diverge in the absence of Pauli limiting, the order parameter corresponding to the weaker of the two pairing interactions is suppressed, allowing the vortex cores to penetrate those layers or interstitials. Although we have not yet solved for the flux lattice structure in such a situation, we anticipate that the flux lattice in a parallel field below T^* with N = 2 will consist of alternating superconducting and normal layers. Such a mixed state should be capable of carrying large currents, since the flux lattice is pinned intrinsically by the crystal lattice.

This work was supported by the U. S. Department of Energy, Division of Basic Energy Sciences, under Contract Nos. DE-AC005-84OR21400 with Martin Marietta Energy Systems, Inc., and W-31-109-ENG-38.

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