Fluctuations, size effects, and superconductivity in the CuO_2 bilayer

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Recently, several experimental groups have found superconducting behavior of one-unit-cell (i.e., one CuO_2 bilayer) thick $YBa_2Cu_3O_7$ films. Using the functional-integral method, we calculate the critical temperature T_c for a system of two CuO_2 planes coupled via a tunneling matrix element that results in Josephson-type coupling. The Coulomb interaction between the two planes is considered via inclusion of quantum phase fluctuations. We take into account the fluctuations of the modulus of the superconducting order parameter in the planes and the fluctuations of the phase difference of the order parameter between the planes. While for samples of infinite size T_c is strictly zero, samples of finite size L yield an effective two-dimensional to zero-dimensional transition at a finite temperature T_c^*, characterized by a jump in the specific heat. We obtain T_c^* as a function of L, Josephson coupling parameter, and Coulomb interaction strength and predict the temperature dependence of the specific heat near T_c^*. Our results are consistent with the T_c^* values observed on the single CuO_2 bilayer.

I. INTRODUCTION

One of the central problems in the theory of the high-temperature superconductors is to what extent the superconducting properties are determined by the two dimensionality of the CuO_2 planes, where the microscopic superconducting mechanism is mostly believed to take place, and how the extension into the third dimension is achieved by the coupling between adjacent CuO_2 planes.

In this context transport measurements on $YBa_2Cu_3O_7/PrBa_2Cu_3O_7$ (YBCO/PBCO) superlattices[1] have reached considerable interest. The authors find a resistive superconducting transition in systems consisting of one-unit-cell (i.e., one CuO_2 bilayer) thick YBCO films separated by up to eight-unit-cell thick nonsuperconducting PBCO films with T_c values of up to ~ 20–30 K. Although it is not overall accepted, many physicists working in this field believe that the YBCO layers in these superlattices are completely decoupled by the PBCO layers.[2] So it seems to be the case that a single two-dimensional (2D) CuO_2 bilayer system can exhibit superconducting behavior. Nevertheless, it should also be noted that some authors find a one-unit-cell thick YBCO film sandwiched between PBCO layers to be nonsuperconducting.[3]

The question now arising is the following: Can the transition into the superconducting state be described by fluctuation effects based on a BCS-like model, or is the transition characterized by fluctuations into Kosterlitz-Thouless-type[4] vortex-antivortex pairs?

One should remember that "conventional" superconductivity with $T_c > 0$ is ruled out for systems with two (or less) dimensions,[5] since long-range order is destroyed by phase fluctuations of the superconducting order parameter (OP) for $T > 0$.[6] Some time ago Hassing and Wilkins[7] obtained similar results. They take into account fluctuations of the superconducting OP up to fourth order in a so-called biquadratic approximation; as a consequence of this procedure they only consider the modulus of the OP. When Hassing and Wilkins calculate the critical temperature T_c, they obtain $T_c \equiv 0$ in two or fewer dimensions. Nevertheless, it is not really clear how the phase fluctuations enter their theory.

Motivated by the experiments, we investigate in this paper the superconducting critical temperature T_c in a system consisting of two mutually coupled CuO_2 planes with BCS-type pairing. Part of this work has been published elsewhere.[8] We take into account fluctuations of the modulus of the superconducting OP in the planes up to fourth order in biquadratic approximation, fluctuations of the phase difference of the superconducting OP between the planes, and the Coulomb interaction between the planes via inclusion of quantum phase fluctuations.

In Sec. II we introduce our basic model Hamiltonian, from which we derive a Ginzburg-Landau-type free-energy functional by a functional-integral transformation; we also include the Coulomb interaction. In Sec. III we calculate the critical temperature T_c of a bilayer system with infinite plane size and show that always $T_c \equiv 0$. Effects of *finite* size L are considered in Sec. IV. Numerical results are given in Sec. V for a choice of parameters suitable for YBCO. In Sec. VI we give a summary and discussion.

II. MODEL HAMILTONIAN AND FREE ENERGY

A. Basic Hamiltonian

Omitting the Coulomb interaction at this point (see Sec. II B), we start with the Hamiltonian

$$H = H_0 + H_P + H_T, \tag{2.1a}$$

with

$$H_0 = \sum_{i=1,2} \sum_{\alpha} \varepsilon_\alpha c^\dagger_{i,\alpha} c_{i,\alpha}, \tag{2.1b}$$

$$H_P = -g \sum_{i=1,2} \sum_{Q} b^\dagger_{i,Q} b_{i,Q}, \tag{2.1c}$$

$$H_T = \sum_{\alpha} (t c^\dagger_{1,\alpha} c_{2,\alpha} + \text{H.c.}). \tag{2.1d}$$

Here, $\alpha \equiv (k, \sigma)$ and $b_Q \equiv \sum_k c_{-k\downarrow} c_{k+Q\uparrow}$. The index i refers to the plane. g and t are the intraplane pairing energy and interplane tunneling matrix element, respectively, which are taken to be constants. H_P describes a BCS-like intralayer pairing and H_T a single-particle interlayer tunneling.

Applying a functional-integral transformation[9] to Eq. (2.1a) and introducing the fourth-order term in the superconducting OP in biquadratic approximation[7] yields the free energy in Ginzburg-Landau form (for details see Appendix A),

$$F_{\text{GL}}[\Delta^{(1)}, \Delta^{(2)}] = F_0 + \sum_{Qm} a_{Qm} \left(\left|\Delta^{(1)}_{Qm}\right|^2 + \left|\Delta^{(2)}_{Qm}\right|^2 \right) + N_0 \kappa_0^2 \sum_{Qm} \left|\Delta^{(1)}_{Qm}\right| \left|\Delta^{(2)}_{Qm}\right| \cos\left(\varphi^{(1)}_{Qm} - \varphi^{(2)}_{Qm} - 2\psi\right), \tag{2.2}$$

with

$$a_{Qm} = \frac{N_0}{2} \left\{ \ln \frac{T}{T_{c0}} + \frac{\pi^2}{4}|m| + \xi_0^2 Q^2 + \kappa_0^2 \right\} + \frac{b_0}{2} \sum_{Q'} \left\langle |\Delta_{Q'0}|^2 \right\rangle \delta_{m0}. \tag{2.3}$$

Here, $\Delta^{(i)}_{Qm} = \left|\Delta^{(i)}_{Qm}\right| \exp\left(i\varphi^{(i)}_{Qm}\right)$, $t = |t| \exp(i\psi)$, $\kappa_0 \equiv |t|/(2\omega_0)$, ω_0 is the BCS cutoff parameter, $b_0 = 7/(8\pi^2)\zeta(3) N_0 \beta^2$, $\beta \equiv 1/(k_B T)$, N_0 is the density of states at the Fermi surface in the normal state, and T_{c0} is the Ginzburg-Landau mean-field critical temperature. One sees that the the pairing term H_P, Eq. (2.1c), and the *single*-particle tunneling term H_T, Eq. (2.1d), lead to a Josephson-type coupling term in the free energy. Equation (2.2) has the form of a Lawrence-Doniach free-energy functional[10] without an external magnetic field.

B. Coulomb interaction

To treat the Coulomb interaction correctly, one has to take into account the quantum-mechanical relation between particle number n and total phase φ,

$$[n, \varphi] = i\hbar; \tag{2.4}$$

i.e., n and φ are conjugate variables. Therefore, in the presence of the Coulomb interaction the free energy contains an additional phase-dependent term,[11]

$$F_C = \frac{\hbar}{\beta V_C} \int_0^{\beta\hbar} d\tau \left| \frac{\partial}{\partial \tau} \left[\varphi^{(1)}(\tau) - \varphi^{(2)}(\tau) \right] \right|^2, \tag{2.5}$$

with $V_C = e^2/(2C)$, where C is the capacitance of the bilayer. Setting $\varphi(\tau) = \sum_m \varphi_m \exp(i\omega_m \tau)$ with $\omega_m = 2\pi m/(\beta\hbar)$, $m = 0, \pm1, \pm2, \ldots$, we get

$$F_C = \sum_{Qm} \frac{4\pi^2 m^2}{\beta^2 V_C} \left(\varphi^{(1)}_{Qm} - \varphi^{(2)}_{Qm} \right)^2. \tag{2.6}$$

Especially, one sees that for the static ($m = 0$) component of the free energy the contribution of the Coulomb interaction is zero.

The total free energy $F[\Delta^{(1)}, \Delta^{(2)}]$ is now given by the sum of Eqs. (2.2) and (2.6).

III. CRITICAL TEMPERATURE IN INFINITE SYSTEMS

We first consider a system with planes of infinite size. The critical temperature T_c is defined as the temperature where the uniform and static fluctuation propagator

$$\left\langle |\Delta_{00}|^2 \right\rangle \equiv \left\langle \left|\Delta^{(1)}_{00}\right|^2 \right\rangle = \left\langle \left|\Delta^{(2)}_{00}\right|^2 \right\rangle = \frac{\int \prod_{Qm} \delta\Delta^{(1)}_{Qm} \, \delta\Delta^{(2)}_{Qm} \left|\Delta^{(1)}_{00}\right|^2 e^{-\beta F}}{\int \prod_{Qm} \delta\Delta^{(1)}_{Qm} \, \delta\Delta^{(2)}_{Qm} \, e^{-\beta F}} \tag{3.1}$$

has a pole.[7] The integrations in Eq. (3.1) run over real and imaginary parts of $\Delta^{(1)}_{Qm}$ and $\Delta^{(2)}_{Qm}$. For $Q \neq 0$ and $m \neq 0$, numerator and denominator cancel. Using F_{GL} of Eq. (2.2) (since $F_C \equiv 0$ for $m = 0$), we get

$$\left\langle |\Delta_{00}|^2 \right\rangle = \frac{2\alpha_0}{\beta N_0 (\alpha_0^2 - \kappa_0^4)}. \tag{3.2}$$

Here, $\alpha_0 \equiv 2a_{00}/N_0$. This result is derived in Appendix B. Therefore, the T_c criterion is $\alpha_0 = \kappa_0^2$ or

$$\ln \frac{T_c}{T_{c0}} + \frac{b_{0c}}{N_0} \sum_{Q'} \left\langle |\Delta_{Q'0}|^2 \right\rangle \Bigg|_{\alpha_0 = \kappa_0^2} = 0, \tag{3.3}$$

with $b_{0c} = b_0(T \to T_c)$. The Q' sum yields

$$\sum_{Q'} \left\langle |\Delta_{Q'0}|^2 \right\rangle = \frac{A}{2\pi} \int_0^{\xi_0^{-1}} dQ' \, Q' \left\langle |\Delta_{Q'0}|^2 \right\rangle = \frac{A}{4\pi \xi_0^2 \beta N_0} \ln \frac{(\alpha_0 + 1)^2 - \kappa_0^4}{\alpha_0^2 - \kappa_0^4} \tag{3.4}$$

(A is the area of one CuO_2 plane; ξ_0 is the in-plane zero-temperature superconducting coherence length). This expression diverges at $\alpha_0 = \kappa_0^2$. As a result, we see that Eq. (3.3) always has the solution

$$T_c \equiv 0, \tag{3.5}$$

independently of the interlayer coupling strength $|t|$, which is contained in κ_0. This result is consistent with Ref. 7. In other words, two mutually coupled 2D systems of infinite size still form a 2D system.

IV. SAMPLES OF FINITE SIZE

The divergency of the Q' sum, Eq. (3.4), appears at the *lower* limit of the integral, $Q' = 0$, corresponding to $L \to \infty$, where L is the size of the system. In real situations (i.e., experiments) one always works with specimens of *finite* size L. And even in very large samples the layers consist of crystallites connected by weak links, which act as superconducting regions of finite size. Of course in such systems one does not have a real thermodynamic limit, and so one cannot expect a true phase transition in a mathematically rigorous sense. But how can one treat these finite systems? The wrong procedure would be to introduce a lower cutoff of the order $\sim 1/L$ in the integral, Eq. (3.4), because T_c is determined through the divergency of the fluctuation propagator at $Q = 0$, and so one must not exclude just the low-Q' components in the Q' sum.

The correct procedure is found in Ref. 7. There exists a temperature T_c^*, given by

$$2\pi\xi_{\text{eff}}(T_c^*) = L. \tag{4.1}$$

Here, $\xi_{\text{eff}}(T)$ is the temperature-dependent in-plane superconducting coherence length, defined for $T \geq T_c^*$. At T_c^* the system undergoes an effective 2D-0D transition. Below T_c^*, the Q' sum Eq. (3.4) is dominated by the $(Q' = 0)$ contribution, and so the sum must not be simply converted to an integral. Approximately, we set

$$\sum_{Q'} \left\langle |\Delta_{Q'0}|^2 \right\rangle \approx \begin{cases} \dfrac{A}{2\pi}\displaystyle\int_0^{\xi_0^{-1}} dQ'\, Q' \left\langle |\Delta_{Q'0}|^2 \right\rangle, \\ T > T_c^*, \\ \left\langle |\Delta_{00}|^2 \right\rangle, \\ T < T_c^*. \end{cases} \tag{4.2}$$

The transition can, for example, be characterized by a jump in the specific heat $C_S(T)$ at T_c^*, which is calculated as

$$C_S(T) = -T\frac{\partial^2 F}{\partial T^2} = T\frac{\partial^2}{\partial T^2}\left(\frac{1}{\beta}\ln \mathcal{Z}\right), \tag{4.3}$$

where $\mathcal{Z}$ is the partition function [the denominator of Eq. (3.1)].

To obtain an equation for T_c^*, we consider the two-particle correlation function[12]

$$\rho_{(2)}(\mathbf{r}) \sim \left\langle \psi_\uparrow^\dagger(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r})\psi_\downarrow(0)\psi_\uparrow(0) \right\rangle, \tag{4.4}$$

which has the asymptotic form $\rho_{(2)}(\mathbf{r}) \sim \exp(-|\mathbf{r}|/\xi_{\text{eff}})$ for $|\mathbf{r}| \to \infty$. This behavior for large $|\mathbf{r}|$ defines ξ_{eff}. $\rho_{(2)}(\mathbf{r})$ can be calculated as[7]

$$\rho_{(2)}(\mathbf{r}) \sim \sum_{Qm} e^{i\mathbf{Q}\cdot\mathbf{r}} \left\langle |\Delta_{Qm}|^2 \right\rangle, \tag{4.5}$$

where $\left\langle |\Delta_{Q0}|^2 \right\rangle$ is given by Eq. (3.2) (replace α_0 by $\alpha_{Q0} = \alpha_0 + \xi_0^2 Q^2$). For $|m| \geq 1$,

$$\left\langle |\Delta_{Qm}|^2 \right\rangle = \frac{6}{5\beta N_0 \alpha_{Qm}} \frac{{}_2F_1\left(1,2;\frac{7}{2};1-\frac{\kappa_m^4}{\alpha_{Qm}^2}\right)}{{}_2F_1\left(1,1;\frac{5}{2};1-\frac{\kappa_m^4}{\alpha_{Qm}^2}\right)} \approx \frac{2}{\beta N_0 \alpha_{Qm}} - \frac{\pi\kappa_m^2}{2\beta N_0 \alpha_{Qm}^2} \tag{4.6}$$

(the calculation can be found in Appendix C). Here, ${}_2F_1(a,b;c;y)$ is the hypergeometric function and the approximations

$${}_2F_1\left(1,2;\frac{7}{2};1-x\right) \approx 5 - \frac{15\pi}{4}\sqrt{x} + O[x], \tag{4.7a}$$

$${}_2F_1\left(1,1;\frac{5}{2};1-x\right) \approx 3 - \frac{3\pi}{2}\sqrt{x} + O[x] \tag{4.7b}$$

for $x \ll 1$ are used. $\kappa_m^2 \equiv k(c_m)\kappa_0^2$ with $c_m = 4\pi^2 m^2/(\beta V_C)$, and the function $k(c)$ is shown in Fig. 1. The asymptotic behavior of $k(c)$ is

$$k(c) \approx \begin{cases} 2c + O\left[c^2\right], & c \ll 1, \\ 1 - \dfrac{1}{4c} + O\left[\dfrac{1}{c^{3/2}}\right], & c \gg 1. \end{cases} \tag{4.8}$$

One sees that the "effective interlayer coupling" $k(c_m)|t|^2$ goes to zero for $c_m \to 0$, i.e., $V_C \to \infty$, and approaches the "bare interlayer coupling" $|t|^2$ for $c_m \to \infty$, i.e., $V_C \to 0$, just as one would naively expect.

Now the T_c^* equation is

$$\ln\frac{T_c^*}{T_{c0}} + \kappa_0^2 + \frac{b_{0c}^*}{N_0}\sum_{Q'}\left\langle |\Delta_{Q'0}|^2 \right\rangle\Bigg|_{\alpha_0=\alpha_c^*} = \alpha_c^*, \tag{4.9}$$

where $b_{0c}^* = b_0(T \to T_c^*)$, and α_c^* is the solution of

$$\frac{\dfrac{\alpha_c^*}{\alpha_c^{*2} - \kappa_0^4} + \displaystyle\sum_{m\geq 1}\left(\frac{2}{\alpha_c^* + \pi^2 m/4} - \frac{\pi k(c_m)\kappa_0^2}{2(\alpha_c^* + \pi^2 m/4)^2}\right)}{\dfrac{\alpha_c^{*2} + \kappa_0^4}{(\alpha_c^{*2} - \kappa_0^4)^2} + \displaystyle\sum_{m\geq 1}\left(\frac{2}{(\alpha_c^* + \pi^2 m/4)^2} - \frac{\pi k(c_m)\kappa_0^2}{(\alpha_c^* + \pi^2 m/4)^3}\right)} = \left(\frac{2\pi\xi_0}{L}\right)^2. \tag{4.10}$$

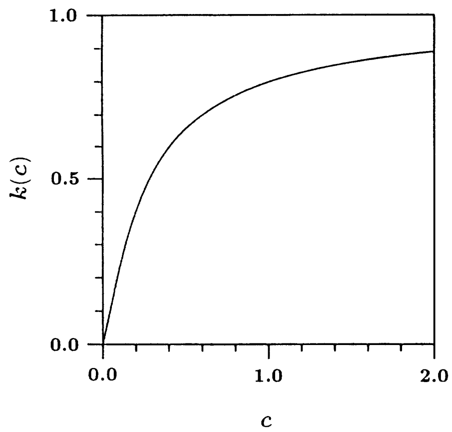

FIG. 1. Function $k(c)$ vs c.

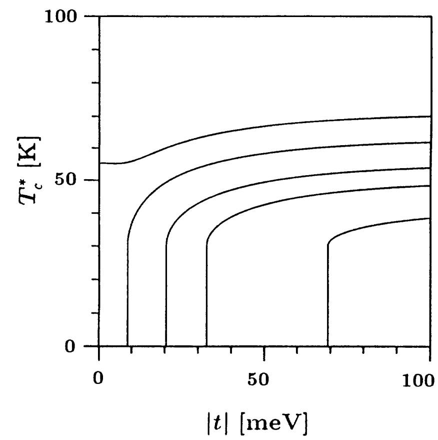

FIG. 3. T_c^* vs $|t|/\omega_0$. From left to right: L = 500, 1000, 2000, 3000, and 5000 Å.

In Appendix D, Eq. (4.10) is derived from Eq. (4.1). In the m sums, only the terms with $m = 1$ are retained, since they yield by far the largest contribution.

V. RESULTS

To obtain quantitative results, we use a set of parameters suitable for YBCO.[13] These are the following: plane separation $d = 3.4$ Å, effective mass $m^* = 6m_0$, $\xi_0 = 15$ Å, $\omega_0 = 50$ meV, and $T_{c0} = 82$ K. The capacitance C is calculated as $C = \varepsilon/(4\pi)A/d$ with $\varepsilon = 4$.

In Fig. 2 we plot T_c^* vs $1/L$ for five different values of $|t|$, and in Fig. 3 we show T_c^* vs $|t|$ for five different values of L with fixed Coulomb interaction strength (see remark below). For each value of $|t|$, there exists a maximum value for L, above which T_c^* is zero. Also, for each L one finds a minimum $|t|$. For small values of L ($2\pi\xi_0/L > 0.2$), T_c^* is approximately linear in $1/L$. Furthermore, our calculations show that the resulting T_c^* values do *not* vary much, if V_C is either very large or very small. The reason for this unexpected behavior is that the Coulomb interaction only affects the ($m \neq 0$) components of Δ, while the ($m = 0$) component makes by far the largest contribution to T_c^*.

In Fig. 4 the superconducting contribution to the specific heat, $C_S(T)$, is plotted vs T in the vicinity of T_c^* for four different L values; the curves are shifted vertically for clarity. One sees that the specific heat jump decreases for increasing L and has almost disappeared for L = 3000 Å.

VI. CONCLUSIONS AND DISCUSSION

In this paper we consider a CuO_2 bilayer system with BCS-type intralayer pairing, single-particle interlayer tunneling (which together leads to Josephson-type coupling terms in the free energy), and interlayer Coulomb interaction via quantum fluctuations of the phase difference of the superconducting OP's in the two planes. We also take into account fluctuations of the modulus of the OP in the planes up to fourth order in a biquadratic approximation. For a system of infinite plane size, we calculate the superconducting critical temperature, which turns out to be always zero, a result consistent with the

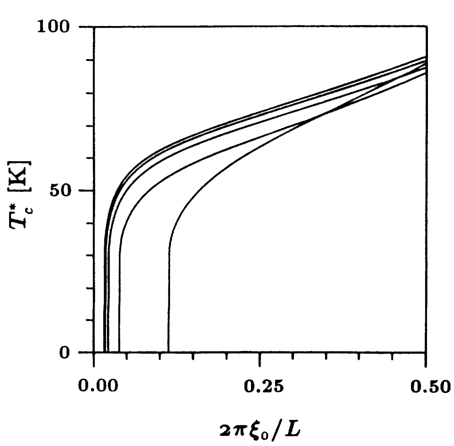

FIG. 2. T_c^* vs $2\pi\xi_0/L$. From right to left: $|t|$ = 0, 25, 50, 75, and 100 meV.

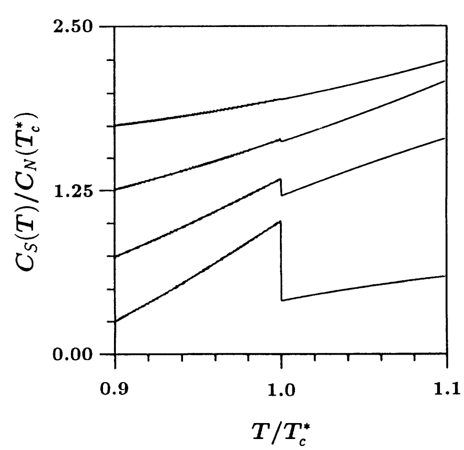

FIG. 4. $C_S(T)$ vs T in the vicinity of T_c^*. From bottom to top: L = 500, 1000, 2000, and 3000 Å.

works of Hohenberg and Rice, due to the strong thermal fluctuations in two-dimensional systems. Then we consider bilayers with finite plane size and obtain a finite temperature T_c^*, where the in-plane superconducting coherence length exceeds the size of the layers and the system undergoes an effective 2D-0D transition. This transition should in principle be measurable by a discontinuity (or at least a rapid change in a finite temperature interval) of the specific heat. Of course, one also expects effects on other quantities, such as the resistivity, but that is not the subject of the present paper and should be studied in further work. With a suitable set of parameters for YBCO, we obtain T_c^* values consistent with experiment, if the measured transition temperatures are identified with our T_c^*'s. Especially, for a realistic value of $|t| = 50$ meV (Ref. 14) we predict that $T_c^* = 0$ for $L > 4500$ Å. Our results turn out to be rather insensitive to the strength of the Coulomb interaction, because all quantities are dominated by the static ($m = 0$) component of Δ, where the Coulomb interaction does not contribute.

Most theoretical work by other authors in this field is done for the case of an infinite number of layers, where it is possible to apply a discrete Fourier transformation in the c direction.[15] A treatment of a system with a finite number of layers is given by Ariosa *et al.*[16] These authors use the well-known XY model to describe the physics *in* the layers and also consider the Coulomb interaction between the layers. They obtain a Kosterlitz-Thouless transition with a transition temperature T_{KT}, which depends on the number of layers via the capacitance of the whole multilayer system. The authors do *not* consider Josephson coupling between the layers.

All these results are in contrast to another group.[17] These authors attribute the variation of the critical temperature with YBCO-layer thickness in the experiments to extrinsic processes, such as charge transfer, at the YBCO/PBCO interfaces and *not* to intrinsic properties of YBCO.

At this point it is not possible to decide whether our model is appropriate to explain the experimental phenomena observed on the YBCO/PBCO superlattices or whether a Kosterlitz-Thouless-type mechanism is responsible for the physical properties. In any case, our results are consistent with experiment. To facilitate a decision about the basic mechanism of superconductivity in the high-T_c oxides, further experiments to clarify the superconducting behavior of one-unit-cell thick YBCO (and also of other high-T_c materials) would be appreciated. It will also be necessary to make more calculations within the framework of our model to obtain a wider set of measurable quantities. A very interesting problem would be a system with more than one but still with a finite number of layers or bilayers. Looking at the experiments, one expects an increasing transition temperature with increasing number of layers and a saturation at the three-dimensional transition temperature for an infinite number of layers. Such a calculation would be a good criterion to check the validity of our model.

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APPENDIX A: GINZBURG-LANDAU FREE-ENERGY FUNCTIONAL

To obtain a free-energy functional, we have to calculate the partition function $\mathcal{Z} = \mathrm{Tr}\, e^{-\beta H}$ with H from Eq. (2.1a). In this appendix, we formally only consider Cooper pairs with zero total momentum ($k\uparrow, -k\downarrow$). We write H as

$$H = \sum_{ij}\sum_{\alpha} \mathsf{A}_{ij} c^\dagger_{i,\alpha} c_{j,\alpha} - g \sum_{i}\sum_{\alpha\alpha'} c^\dagger_{i,\alpha} c^\dagger_{i,\tilde{\alpha}} c_{i,\tilde{\alpha}'} c_{i,\alpha'}, \quad \text{(A1)}$$

where

$$\mathsf{A} = \begin{pmatrix} \varepsilon_\alpha & t \\ t^* & \varepsilon_\alpha \end{pmatrix} \quad \text{(A2)}$$

is a Hermitian matrix, $\alpha = (k,\uparrow)$, and $\tilde{\alpha} = (-k,\downarrow)$. Now one has to introduce two complex random variables ζ_1 and ζ_2 to get rid of the four-c term in H and to get an expression for $\mathcal{Z}$ which only contains products of two c operators. Later, ζ_1 and ζ_2 will turn out to be proportional to the gaps in the two layers, $\Delta^{(1)}$ and $\Delta^{(2)}$. In the static limit, where ζ_1 and ζ_2 are time independent, $\mathcal{Z}$ can be written as[9]

$$\mathcal{Z} = \int \delta\zeta_1\, \delta\zeta_2\, e^{-\pi(|\zeta_1|^2+|\zeta_2|^2)} \times \prod_{\alpha} \mathrm{Tr}\, \exp\left(-\beta \sum_{ij} \left\{ \mathsf{A}_{ij} c^\dagger_{i,\alpha} c_{j,\alpha} + \frac{1}{2}\mathsf{B}_{ij}(c^\dagger_{i,\alpha} c^\dagger_{j,\tilde{\alpha}} - c^\dagger_{i,\tilde{\alpha}} c^\dagger_{j,\alpha}) + \frac{1}{2}\mathsf{B}^*_{ij}(c_{i,\tilde{\alpha}} c_{j,\alpha} - c_{i,\alpha} c_{j,\tilde{\alpha}}) \right\}\right), \quad \text{(A3)}$$

where

$$\mathsf{B} = -\sqrt{\frac{\pi g}{\beta}} \begin{pmatrix} \zeta_1 & 0 \\ 0 & \zeta_2 \end{pmatrix} \quad \text{(A4)}$$

is a symmetric matrix.

To perform the trace, we have to bring the sum $\sum_{ij}\{\cdots\}$ in Eq. (A3) into the form

$$\sum_{i=1}^{2}\lambda_{i,\alpha}\eta_{i,\alpha}^{\dagger}\eta_{i,\alpha}+\text{const}, \tag{A5}$$

where the η's are Fermi operators. This is done with a procedure similar to calculations by Lieb *et al.*[18] Our aim is to diagonalize an operator of the form

$$\mathcal{O}=\sum_{ij}\left[\mathsf{A}_{ij}c_i^{\dagger}c_j+\frac{1}{2}\mathsf{B}_{ij}\left(c_{i\uparrow}^{\dagger}c_{j\downarrow}^{\dagger}-c_{i\downarrow}^{\dagger}c_{j\uparrow}^{\dagger}\right)+\frac{1}{2}\mathsf{B}_{ij}^{*}\left(c_{i\downarrow}c_{j\uparrow}-c_{i\uparrow}c_{j\downarrow}\right)\right], \tag{A6}$$

with $\mathsf{A}_{ij}=\mathsf{A}_{ji}^{*}$ and $\mathsf{B}_{ij}=\mathsf{B}_{ji}$. We make the ansatz

$$\eta_{k\uparrow}=\sum_{m}\left(g_{km}c_{m\uparrow}+h_{km}c_{m\downarrow}^{\dagger}\right). \tag{A7}$$

With help of the relation $[\mathcal{A},\mathcal{BC}]=\{\mathcal{A},\mathcal{B}\}\mathcal{C}-\mathcal{B}\{\mathcal{A},\mathcal{C}\}$, where $[\cdots]$ and $\{\cdots\}$ denote commutator and anticommutator, respectively, we get

$$\begin{aligned}[\eta_{k\uparrow},\mathcal{O}]&=\sum_{mj}\left(g_{km}\mathsf{A}_{mj}c_{j\uparrow}+g_{km}\mathsf{B}_{mj}c_{j\downarrow}^{\dagger}-h_{km}\mathsf{A}_{mj}^{*}c_{j\downarrow}^{\dagger}+h_{km}\mathsf{B}_{mj}^{*}c_{j\uparrow}\right)\\&=\lambda_k\eta_{k\uparrow}\\&=\sum_{j}\left(\lambda_k g_{kj}c_{j\uparrow}+\lambda_k h_{kj}c_{j\downarrow}^{\dagger}\right).\end{aligned} \tag{A8}$$

Comparison yields the matrix equations

$$\lambda_k\mathbb{1}\cdot\mathbf{g}_k=\mathsf{A}\cdot\mathbf{g}_k+\mathsf{B}^{*}\cdot\mathbf{h}_k, \tag{A9a}$$

$$\lambda_k\mathbb{1}\cdot\mathbf{h}_k=\mathsf{B}\cdot\mathbf{g}_k-\mathsf{A}^{*}\cdot\mathbf{h}_k, \tag{A9b}$$

which lead to

$$\left[\mathsf{B}^{*}\cdot(\mathsf{A}^{*}+\lambda_k\mathbb{1})^{-1}\cdot\mathsf{B}+\mathsf{A}-\lambda_k\mathbb{1}\right]\cdot\mathbf{g}_k=0. \tag{A10}$$

Here, $\mathbb{1}$ denotes the unit matrix. A nontrivial solution of Eq. (A10) only exists if

$$\det\left[\mathsf{B}^{*}\cdot(\mathsf{A}^{*}+\lambda_k\mathbb{1})^{-1}\cdot\mathsf{B}+\mathsf{A}-\lambda_k\mathbb{1}\right]=0. \tag{A11}$$

Equation (A11) is used to determine the λ's of Eq. (A5). Inserting our matrices A and B, Eqs. (A2) and (A4), and setting $\sqrt{\pi g/\beta}\zeta_{1,2}=\Delta_{1,2}$, we obtain the solutions ($\mu=1$, 2)

$$\begin{aligned}\lambda_{\mu,\alpha}^2=&\ \varepsilon_\alpha^2+\frac{1}{2}|\Delta_1|^2+\frac{1}{2}|\Delta_2|^2+|t|^2\\&\pm\frac{1}{2}\Big[\left(|\Delta_1|^2-|\Delta_2|^2\right)^2\\&+4|t|^2\{4\varepsilon_\alpha^2+|\Delta_1|^2+|\Delta_2|^2\\&-2|\Delta_1||\Delta_2|\cos(\varphi_1-\varphi_2-2\psi)\}\Big]^{1/2},\end{aligned} \tag{A12}$$

where the upper (lower) sign corresponds to $\mu=1$ (2). The symbols are explained below Eq. (2.3). Now the trace in Eq. (A3) can be performed, since the expectation values of the operators $\eta^{\dagger}\eta$ are only 0 and 1. The result is

$$\begin{aligned}\mathcal{Z}=&\left(\frac{\beta}{\pi g}\right)^2\int\delta\Delta_1\,\delta\Delta_2\,e^{-\beta/g(|\Delta_1|^2+|\Delta_2|^2)}\\&\times\prod_{\alpha}\exp\left(-\beta\left\{\varepsilon_\alpha-\frac{1}{2}\lambda_{1,\alpha}-\frac{1}{2}\lambda_{2,\alpha}\right\}\right)\\&\times\left(1+e^{-\beta\lambda_{1,\alpha}}\right)\left(1+e^{-\beta\lambda_{2,\alpha}}\right).\end{aligned} \tag{A13}$$

We now introduce $\mathcal{Z}_0$, the partition function in the normal state, and write

$$\frac{\mathcal{Z}_0}{\mathcal{Z}_0}\equiv\left(\frac{\beta}{\pi g}\right)^2\int\delta\Delta_1\,\delta\Delta_2\,e^{-\beta F[\Delta_1,\Delta_2]}, \tag{A14}$$

with

$$\begin{aligned}F[\Delta_1,\Delta_2]=&\frac{|\Delta_1|^2}{g}+\frac{|\Delta_2|^2}{g}\\&+\sum_{\alpha}\Big\{\varepsilon_\alpha-\frac{1}{2}\lambda_{1,\alpha}-\frac{1}{2}\lambda_{2,\alpha}\\&+\frac{2}{\beta}\ln\left(1+e^{-\beta\varepsilon_\alpha}\right)-\frac{1}{\beta}\ln\left(1+e^{-\beta\lambda_{1,\alpha}}\right)\\&-\frac{1}{\beta}\ln\left(1+e^{-\beta\lambda_{2,\alpha}}\right)\Big\}.\end{aligned} \tag{A15}$$

The next step is to expand λ_1 and λ_2 up to order $|t|^2$,

$$\begin{aligned}\lambda_{1,\alpha}\approx&\sqrt{\varepsilon_\alpha^2+|\Delta_1|^2}+\frac{|t|^2}{\sqrt{\varepsilon_\alpha^2+|\Delta_1|^2}}\\&\times\frac{2\varepsilon_\alpha^2+|\Delta_1|^2-|\Delta_1||\Delta_2|\cos\tilde{\varphi}}{|\Delta_1|^2-|\Delta_2|^2},\end{aligned} \tag{A16}$$

with $\tilde{\varphi}\equiv\varphi_1-\varphi_2-2\psi$ and $\lambda_{2,\alpha}=\lambda_{1,\alpha}$ with $|\Delta_1|\leftrightarrow|\Delta_2|$. Replacing the sum over α by an integral over ε_α,

$$\sum_{\alpha}\to2N_0\int_0^{\omega_0}d\varepsilon_\alpha, \tag{A17}$$

and integrating, we get, up to second order in the OP's,

$$F = \frac{N_0}{2}\left(|\Delta_1|^2 + |\Delta_2|^2\right)\ln\frac{T}{T_{c0}} - N_0|t|^2 + \frac{N_0|t|^2}{8\omega_0^2}\left(|\Delta_1|^2 + |\Delta_2|^2\right) + \frac{N_0|t|^2}{4\omega_0^2}|\Delta_1||\Delta_2|\cos(\varphi_1 - \varphi_2 - 2\psi). \quad \text{(A18)}$$

A generalization of Eq. (A18) to finite Q and m values and introduction of the fourth order term in Δ according to Ref. 7 leads to Eq. (2.2).

APPENDIX B: STATIC AND UNIFORM FLUCTUATION PROPAGATOR

We have to calculate an expression of the form

$$\frac{I_{\rm num}}{I_{\rm den}} = \frac{\int_0^\infty dx_1\, x_1^3 \int_0^\infty dx_2\, x_2 \int_{-\pi}^{+\pi} d\varphi_1 \int_{-\pi}^{+\pi} d\varphi_2\, e^{-a(x_1^2+x_2^2)-\gamma x_1 x_2 \cos(\varphi_1-\varphi_2-2\psi)}}{\int_0^\infty dx_1\, x_1 \int_0^\infty dx_2\, x_2 \int_{-\pi}^{+\pi} d\varphi_1 \int_{-\pi}^{+\pi} d\varphi_2\, e^{-a(x_1^2+x_2^2)-\gamma x_1 x_2 \cos(\varphi_1-\varphi_2-2\psi)}}. \quad \text{(B1)}$$

With the substitution $\theta = \varphi_1 - \varphi_2 - 2\psi$, the angle integration yields[19]

$$\int_{-\pi}^{+\pi} d\varphi_2 \int_{-\pi-\varphi_2-2\psi}^{+\pi-\varphi_2-2\psi} d\theta\, e^{-\gamma x_1 x_2 \cos\theta} = (2\pi)^2 I_0(\gamma x_1 x_2), \quad \text{(B2)}$$

where I_0 is a modified Bessel function of order zero. The x_2 integration then is[19]

$$\int_0^\infty dx_2\, x_2\, I_0(\gamma x_1 x_2)\, e^{-a x_2^2} = \frac{1}{2a} e^{\gamma^2 x_1^2/(4a)}. \quad \text{(B3)}$$

Finally,

$$I_{\rm num} \propto \int_0^\infty dx_1\, x_1^3\, e^{-[a-\gamma^2/(4a)]x_1^2} = \frac{1}{2\left[a - \gamma^2/(4a)\right]^2} \quad \text{(B4)}$$

and

$$I_{\rm den} \propto \int_0^\infty dx_1\, x_1\, e^{-[a-\gamma^2/(4a)]x_1^2} = \frac{1}{2\left[a - \gamma^2/(4a)\right]}, \quad \text{(B5)}$$

so that

$$\frac{I_{\rm num}}{I_{\rm den}} = \frac{1}{a - \gamma^2/(4a)}. \quad \text{(B6)}$$

With $a = \beta a_{00} \equiv \beta N_0 \alpha_0/2$ and $\gamma = \beta N_0 \kappa_0^2$, we obtain Eq. (3.2).

APPENDIX C: FLUCTUATION PROPAGATOR WITH COULOMB INTERACTION

We first consider the phase-dependent term of the free energy, $F^\varphi = \sum_{Qm} F^\varphi_{Qm}$, with

$$F^\varphi_{Qm} = \frac{4\pi^2 m^2}{\beta^2 V_C}\left(\varphi^{(1)}_{Qm} - \varphi^{(2)}_{Qm}\right)^2 + N_0\kappa_0^2 \left|\Delta^{(1)}_{Qm}\right| \left|\Delta^{(2)}_{Qm}\right| \cos\left(\varphi^{(1)}_{Qm} - \varphi^{(2)}_{Qm}\right). \quad \text{(C1)}$$

For fixed Q and m, we have to calculate

$$I^\varphi_{Qm} \equiv \int_{-\pi}^{+\pi} d\varphi^{(1)}_{Qm} \int_{-\pi}^{+\pi} d\varphi^{(2)}_{Qm}\, e^{-\beta F^\varphi_{Qm}}. \quad \text{(C2)}$$

In the following, we suppress the indices Q and m. Since F^φ only depends on the phase *difference*, we substitute

$$\varphi_1 - \varphi_2 = \phi, \quad \text{(C3a)}$$

$$\varphi_1 + \varphi_2 = \psi, \quad \text{(C3b)}$$

$$d\varphi_1\, d\varphi_2 = \frac{1}{2}\, d\phi\, d\psi. \quad \text{(C3c)}$$

The regions of integration for the phase variables φ_1, φ_2 and ϕ, ψ are sketched in Fig. 5. For any even function f that only depends on ϕ we get

$$\int_{-\pi}^{+\pi} d\varphi_1 \int_{-\pi}^{+\pi} d\varphi_2\, f(\phi) = \int_0^{2\pi} d\phi\, (4\pi - 2\phi)\, f(\phi). \quad \text{(C4)}$$

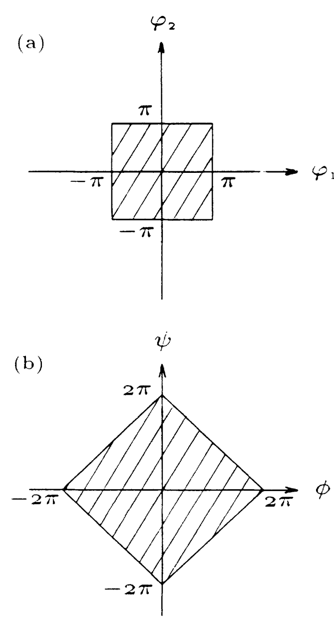

FIG. 5. Regions of integration for the phase integrations (a) in the variables φ_1 and φ_2, (b) in the variables ϕ and ψ.

So we now have to evaluate integrals of the form

$$4\pi \int_0^{2\pi} d\phi\, e^{-c\phi^2 - d\cos\phi} - 2\int_0^{2\pi} d\phi\,\phi\, e^{-c\phi^2 - d\cos\phi}, \quad \text{(C5)}$$

with

$$c \equiv c_m = \frac{4\pi^2 m^2}{\beta V_C}, \quad \text{(C6a)}$$

$$d = \underbrace{\beta N_0 \kappa_0^2}_{\gamma} |\Delta_1||\Delta_2|, \quad \text{(C6b)}$$

which cannot be done directly. Instead, we use the series expansion[19]

$$e^{-d\cos\phi} = I_0(d) + 2\sum_{k=1}^{\infty}(-1)^k I_k(d)\cos k\phi, \quad \text{(C7)}$$

where the I_k are modified Bessel functions of order k. If we insert Eq. (C7) into Eq. (C2), we have

$$I^{\varphi} = \sum_{k=0}^{\infty} A_k(c) I_k(d), \quad \text{(C8)}$$

with

$$A_0(c) = 4\pi \int_0^{2\pi} d\phi\, e^{-c\phi^2} - 2\int_0^{2\pi} d\phi\,\phi\, e^{-c\phi^2}, \quad \text{(C9a)}$$

$$A_k(c) = (-1)^k \left(8\pi \int_0^{2\pi} d\phi\, e^{-c\phi^2}\cos k\phi - 4\int_0^{2\pi} d\phi\,\phi\, e^{-c\phi^2}\cos k\phi\right) \text{ for } k \geq 1. \quad \text{(C9b)}$$

To get rid of the infinite sum over k, we write I^{φ} in the form

$$\exp\ln I^{\varphi} = \exp\ln \sum_{k=0}^{\infty} A_k(c) I_k(d) \quad \text{(C10)}$$

and expand the logarithm up to the second order in d, i.e., to order $|\Delta_1||\Delta_2|$, so that the integrand of the $|\Delta_1|$ and $|\Delta_2|$ integrations has the form $e^{-\beta\tilde{F}}$, where $\tilde{F}$ contains the Josephson coupling terms up to quadratic order in $|\Delta|$. Taking into account the behavior of the Bessel functions at small arguments, one gets

$$\ln \sum_{k=0}^{\infty} A_k(c) I_k(d) \approx \ln A_0(c) - k(c)d + O\left[d^2\right], \quad \text{(C11)}$$

with

$$k(c) = -\frac{A_1(c)}{2A_0(c)} \quad \text{(C12)}$$

$[k(c) \geq 0$, since $A_1(c) \leq 0]$. Especially, one sees that only a finite number of A_k functions contribute to the expansion coefficients. The term $\ln A_0(c)$ is independent of $|\Delta_1|$ and $|\Delta_2|$ and is absorbed in F_0. In presence of the Coulomb interaction, the "effective" interlayer coupling is given by $k(c)|t|^2$ (d is proportional to $|t|^2$). The function $k(c)$ is plotted in Fig. 1.

We now examine the asymptotic behavior of $k(c)$. For large c, we can replace the upper limit of integration in Eqs. (C9) by ∞. Then,[19]

$$A_0(c) \approx \frac{2\pi^{3/2}}{\sqrt{c}} - \frac{1}{c}, \quad \text{(C13a)}$$

$$A_1(c) \approx -\frac{4\pi^{3/2}}{\sqrt{c}} e^{-1/(4c)} + \frac{2}{c} - \frac{1}{c^2}\sum_{n=0}^{\infty}\frac{(-1)^n n!}{(2n+1)! c^n}. \quad \text{(C13b)}$$

For small c,

$$A_0(c) \approx 4\pi^2 - \frac{8\pi^4}{3}c + O\left[c^2\right], \quad \text{(C14a)}$$

$$A_1(c) \approx -16\pi^2 c + O\left[c^2\right]. \quad \text{(C14b)}$$

Equation (4.8) then follows from Eqs. (C13) and (C14).

To perform the remaining integrations over $|\Delta_1|$ and $|\Delta_2|$, one has to evaluate integrals of the form

$$\int_0^{\infty} dx_1 \begin{Bmatrix} x_1^3 \\ x_1 \end{Bmatrix} \int_0^{\infty} dx_2\, x_2\, e^{-a(x_1^2+x_2^2)-\lambda x_1 x_2}, \quad \text{(C15)}$$

with $\lambda = \beta k(c)\gamma$. The x_2 integration yields[19]

$$\frac{1}{2a}\Gamma(2) e^{\lambda^2 x_1^2/(8a)} D_{-2}\left(\frac{\lambda x_1}{\sqrt{2a}}\right), \quad \text{(C16)}$$

where D_{-2} is a parabolic cylinder function. Finally,[19]

$$\int_0^{\infty} dx_1\, x_1^3\, e^{-[a-\lambda^2/(8a)]x_1^2} D_{-2}\left(\sqrt{\frac{\lambda^2}{2a}}x_1\right) = \frac{2^{-4}\sqrt{\pi}\Gamma(4)}{2\Gamma(7/2)a^2}\, {}_2F_1\left(1,2;\frac{7}{2};\frac{a-\lambda^2/(4a)}{a}\right) \quad \text{(C17)}$$

and

$$\int_0^{\infty} dx_1\, x_1\, e^{-[a-\lambda^2/(8a)]x_1^2} D_{-2}\left(\sqrt{\frac{\lambda^2}{2a}}x_1\right) = \frac{2^{-2}\sqrt{\pi}\Gamma(2)}{2\Gamma(5/2)a}\, {}_2F_1\left(1,1;\frac{5}{2};\frac{a-\lambda^2/(4a)}{a}\right), \quad \text{(C18)}$$

from which Eq. (4.6) immediately follows.

APPENDIX D: DERIVATION OF Eq. (4.10)

To obtain an expression for ξ_{eff}, we have to calculate

$$\sum_{Qm} e^{i\mathbf{Q}\cdot\mathbf{r}} \left\langle |\Delta_{Qm}|^2 \right\rangle; \quad \text{(D1)}$$

cf. Eq. (4.5). For $m = 0$, we get, with help from Eq. (3.2),

$$\left\langle |\Delta_{Q0}|^2 \right\rangle = \frac{2\alpha_{Q0}}{\beta N_0(\alpha_{Q0}^2 - \kappa_0^4)} \equiv \frac{2(\alpha_0 + \xi_0^2 Q^2)}{\beta N_0[(\alpha_0 + \xi_0^2 Q^2)^2 - \kappa_0^4]}. \quad \text{(D2)}$$

For $m \geq 1$ we write α_{Qm} as

$$\alpha_{Qm} \equiv \alpha_0 + B_m + \xi_0^2 Q^2, \qquad \text{(D3)}$$

with

$$B_m = \frac{\pi^2}{4}|m| - \frac{b_0}{N_0} \sum_{Q'} \left\langle |\Delta_{Q'0}|^2 \right\rangle, \qquad \text{(D4)}$$

and since always $\alpha_{Qm} > 1$ for $m \geq 1$, we use the approximation in the second line of Eq. (4.6). Furthermore, we have

$$\sum_{m=0,\pm1,\ldots} \left\langle |\Delta_{Qm}|^2 \right\rangle = \left\langle |\Delta_{Q0}|^2 \right\rangle + 2 \sum_{m\geq1} \left\langle |\Delta_{Qm}|^2 \right\rangle, \quad \text{(D5)}$$

since the argument of the sum only depends on $|m|$.

If we had no interlayer coupling, i.e., $\kappa_0 \equiv 0$, the function to be Fourier transformed in Eq. (4.5) would just be proportional to $(\alpha_0 + \xi_0^2 Q^2)^{-1}$. Since ξ_{eff} is determined by the large $|\mathbf{r}|$, i.e., small Q behavior of the correlation function, we expand $\left(\sum_m \left\langle |\Delta_{Qm}|^2 \right\rangle\right)^{-1}$ up to quadratic order in Q and bring it into the form $B(Q)^{-1} \equiv \delta_1(1+\delta_2\xi_0^2 Q^2)$. The Fourier transformation then yields[19]

$$\begin{aligned}\sum_Q e^{i\mathbf{Q}\cdot\mathbf{r}} B(Q) &\propto \int_0^\infty dQ\, Q \int_0^{2\pi} d\vartheta\, e^{iQr\cos\vartheta} B(Q) \\ &\propto \int_0^\infty dQ\, \frac{Q}{\delta_1(1+\delta_2\xi_0^2 Q^2)} J_0(rQ) \\ &\propto \int_0^\infty dQ\, \frac{Q}{(\sqrt{\delta_2}\xi_0)^{-2} + Q^2} J_0(rQ) \\ &= K_0\left(\frac{r}{\sqrt{\delta_2}\xi_0}\right), \end{aligned} \qquad \text{(D6)}$$

where J_0 and K_0 are again Bessel functions of order zero. The asymptotic behavior of $K_0(z)$ for large z is[19]

$$K_0(z) \approx \sqrt{\frac{\pi}{2z}} e^{-z} \left(1 + O\left[\frac{1}{z}\right]\right), \qquad \text{(D7)}$$

so that

$$\xi_{\text{eff}} \equiv \sqrt{\delta_2}\xi_0 \qquad \text{(D8)}$$

is identified with the effective superconducting coherence length. Thus we have to determine δ_2. Expanding $\sum_m \left\langle |\Delta_{Qm}|^2 \right\rangle$ in Q, we get

$$\delta_2 = \frac{\dfrac{\alpha_0}{\alpha_0{}^2 - \kappa_0^4} + \sum_{m\geq1}\left(\dfrac{2}{\alpha_0 + B_m} - \dfrac{\pi k(c_m)\kappa_0^2}{2(\alpha_0+B_m)^2}\right)}{\dfrac{\alpha_0{}^2 + \kappa_0^4}{(\alpha_0{}^2 - \kappa_0^4)^2} + \sum_{m\geq1}\left(\dfrac{2}{(\alpha_0+B_m)^2} - \dfrac{\pi k(c_m)\kappa_0^2}{(\alpha_0+B_m)^3}\right)}. \qquad \text{(D9)}$$

Now α_c^* is defined by Eq. (4.1) at $\alpha_0 = \alpha_c^*$, which leads to Eq. (4.10), if we set B_m approximately equal to $\pi^2 m/4$. Numerically this turns out to be a good approximation.

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