Temperature dependence of specific heat and penetration depth of anisotropic-gap Bardeen-Cooper-Schrieffer superconductors for a factorizable pairing potential

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An explicit expression for the temperature dependence of the specific heat of clean anisotropic-gap superconductors is derived within the weak-coupling BCS approximation. The specific heat is presented as a functional of the superconducting gap on the Fermi surface. The obtained formula interpolates between the correct low coupling jump at T_c and the low-temperature behavior for $T \ll T_c$. For isotropic superconductors, the formula gives a relation between the specific heat and the superconducting gap. For anisotropic superconductors, the interpolation formula incorporates averaging of powers of the gap anisotropy function over the Fermi surface and provides a suitable set for fitting model Hamiltonians to experimental data. The work of the interpolation formula is illustrated by (i) the Pokrovsky formula for the specific heat jump; (ii) Gor'kov and Melik-Barkhudarov formulas for the Ginzburg-Landau coefficients; (iii) the Moskalenko two-band formula for the specific heat jump; (iv) the temperature dependence of the specific heat for the two-band model, applicable to MgB_2; (v) the two-dimensional *d*-wave model, applicable for $YBa_2Cu_3O_{7-\delta}$; and (vi) the Zhitomirsky and Rice triplet *p*-wave model with horizontal line nodes for Sr_2RuO_4. The temperature dependence of the penetration depth is illustrated by fitting the general theoretical formula to the experimental data for MgB_2, $YBa_2Cu_3O_{7-\delta}$, and the triplet superconductor Sr_2RuO_4.

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I. SPECIFIC HEAT

Virtually all recently studied superconductors exhibit considerable anisotropy of the superconducting gap $\Delta_p(T)$ over the Fermi surface $\varepsilon_p = E_F$. Despite the strong-coupling effects and influence of disorder, which are all essential as a rule, for a qualitative analysis it is particularly useful to start with the weak-coupling BCS approximation for clean superconductors. In this case, very often model factorizable pairing potentials give an acceptable accuracy for the preliminary analysis of the experimental data.

The aim of the present work is twofold. First, we shall derive an explicit interpolation formula for the temperature dependence of the specific heat $C(T)$. The formula is formally exact for factorizable pairing kernels, which are a consequence of the approximative separation in the superconducting order parameter derived in the BCS weak-coupling approximation by Pokrovskii.[1] Our formula reproduces the specific heat jump derived by Pokrovskii[1] for arbitrary weak-coupling kernels and Gor'kov and Melik-Barkhudarov[2] results for the Ginzburg-Landau (GL) coefficients of an anisotropic superconductor. That is why we believe that the suggested formula can be useful for the analysis of experimental data when only gap anisotropy and band structure are known. Second, within the same system of notions, we present the recent results by Kogan[3] for the penetration depth $\lambda(T)$ and propose for the zero-scattering case formulas that may be used for experimental data processing.

We begin with the entropy of a Fermi system per unit volume divided by the Boltzmann's constant k_B

$$S(T) = -2\overline{n_p \ln n_p + (1-n_p)\ln(1-n_p)}, \tag{1}$$

where the factor 2 takes into account the spin degeneracy and the overline denotes integration over the *D*-dimensional momentum space

$$\overline{f_p} = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \frac{d^D p}{(2\pi\hbar)^D} f(\mathbf{p}). \tag{2}$$

The Fermi filling factors of independent Fermions

$$n_p = \frac{1}{\exp(2z_p)+1}, \quad z_p \equiv \frac{E_p}{2T}, \tag{3}$$

where T is the temperature times k_B, are expressed by spectrum of superconductor

$$E_p = \sqrt{\xi_p^2 + |\Delta_p|^2}, \quad \xi_p = \varepsilon_p - E_F. \tag{4}$$

Here we have to emphasize that for a model factorizable pairing potential $V_{p,q} \propto \chi_p \chi_q$ the gap function is always separable as a product of a temperature-dependent function that can be associated with the GL order parameter $Q(T)$ and a rigid temperature-independent function of the momentum χ_p. The nontrivial result[1] is that this separation of the variables is asymptotically correct in the BCS weak-coupling limit for an arbitrary kernel, which is generally nonfactorizable. In fact, a factorizable kernel is a fairly unnatural property that, however, can occur if the pairing interaction is local, intraatomic, and located in a single atom in the unit cell. This is the special case of the *s-d* interaction at the copper site(s) in

the CuO_2 plane.[4] The separability ansatz, though, shall be employed here to obtain a general interpolation formula formally exact for factorizable kernels. We assume that the gap anisotropy function χ_p is known either as a result of solving the general BCS equation at T_c, inferred from experimental data processing, or merely postulated within some model Hamiltonian, which is often the case for the high-temperature and exotic superconductors.

With the above remarks, we will derive $C(T)$ for the separable gap

$$\Delta_p(T) = Q(T)\chi_p \tag{5}$$

and a factorizable kernel.[5] We apply the ansatz (5) to the BCS gap equation[6]

$$\Delta_p(T) = \int \frac{d^D q}{(2\pi\hbar)^D} V_{p,q} \frac{1-2n_q}{2E_q} \Delta_q(T), \tag{6}$$

and use the convention that a positive sign of $V_{p,q}$ corresponds to the attraction of charge carriers and a negative potential energy of interaction. Substituting here

$$V_{p,q} \approx G\chi_p\chi_q \tag{7}$$

and introducing $\eta \equiv |Q|^2$, we obtain a transcendental equation for the temperature dependence of the gap $Q(T)$

$$GA(\eta,T) = 1,$$

$$A(\eta,T) \equiv \overline{\left(\frac{\chi_p^2 \tanh z_p}{2E_p}\right)}, \tag{8}$$

where we have used the identity $1-2n_p = \tanh z_p$ and the coupling constant is defined by $G \equiv 1/A(0,T_c)$. Details on the derivation of the trial function approximation [Eq. (7)] and the numerical solution of Eq. (8) for $T_c \ll \omega_D$ are given in Appendix A.

For the specific heat of the superconducting phase per unit volume divided by k_B we have

$$C(T) = Td_T S(\eta(T),T) = 2\overline{E_p d_T n_p} = C_\nu + C_\Delta, \tag{9}$$

where $d_T = d/dT$. Here C_ν is the "normal" part of the specific heat

$$C_\nu(T) \equiv T(\partial_T S)_\eta = \frac{\pi^2}{3}\overline{g_c(z_p)}, \tag{10}$$

where

$$g_c(z) \equiv \frac{6}{\pi^2}\frac{z^2}{\cosh^2 z}, \quad \int_{-\infty}^{\infty} g_c(z)dz = 1, \tag{11}$$

and $(\partial_T \ldots)_\eta$ is the temperature differentiation for the constant-order parameter. For zero-order parameter, $\eta = 0$ at T_c and above, C_ν is just the specific heat of the normal phase $C_N(T) = C_\nu(T, \eta = 0)$.

Introducing

$$\alpha(\eta,T) \equiv -(\partial_T A)_\eta = -(\partial_\eta S)_T = \frac{\overline{\chi_p^2 g_a(z_p)}}{2T^2}, \tag{12}$$

where

$$g_a(z) \equiv \frac{1}{2\cosh^2 z}, \quad \int_{-\infty}^{\infty} g_a(z)dz = 1, \tag{13}$$

the other term of the specific heat

$$C_\Delta \equiv T\partial_\eta S(\eta,T) d_T \eta(T) \tag{14}$$

can be written as

$$C_\Delta = \alpha(\eta,T)[-d_T\eta(T)]\theta(T_c - T). \tag{15}$$

Equation (12) is actually a Maxwell-type equation $\partial_\eta \partial_T F = \partial_T \partial_\eta F$, where F is the free energy: $S = -(\partial_T F)_\eta$ and $A = -(\partial_\eta F)_T$; cf. Ref. 7.

Differentiating Eq. (8) we obtain $dA = 0$ and

$$-d_T\eta(T) = \left.\frac{(\partial_T A)_\eta}{(\partial_\eta A)_T}\right|_{\eta(T)} = \left.\frac{\alpha}{b}\right|_{\eta(T)}, \tag{16}$$

where the functions α and b represent a generalization of the GL coefficients for arbitrary temperature and order parameter

$$b(\eta,T) \equiv -(\partial_\eta A)_T = \frac{7\zeta(3)}{16\pi^2 T^3}\overline{\chi_p^4 g_b(z_p)}, \tag{17}$$

$$g_b(z) \equiv \frac{\pi^2}{14\zeta(3)}\frac{1}{z^2}\left(\frac{\tanh z}{z} - \frac{1}{\cosh^2 z}\right), \tag{18}$$

$$\int_{-\infty}^{\infty} g_b(z)dz = 1, \tag{19}$$

and ζ is the Riemann zeta function. Then

$$C_\Delta = T\frac{\alpha^2}{b} = \frac{4\pi^2}{7\zeta(3)}\frac{[\overline{\chi_p^2 g_a(z_p)}]^2}{\overline{\chi_p^4 g_b(z_p)}}\theta(T_c - T) \tag{20}$$

and

$$\frac{C_\Delta}{C_\nu} = \frac{12}{7\zeta(3)}\frac{[\overline{\chi_p^2 g_a(z_p)}]^2}{\overline{\chi_p^4 g_b(z_p)}\,\overline{g_c(z_p)}}\theta(T_c - T). \tag{21}$$

The functions $g_i(z_p)$, $i = a,b,c$, introduced in Refs. 7 and 8, have sharp maximum at the Fermi surface and in a good approximation we have

$$\overline{\chi_p^n g_i(z_p)} \approx 2T\nu_F\langle\chi_p^n r_i(y_p)\rangle, \quad y_p \equiv \frac{\Delta_p}{2T}, \tag{22}$$

where

$$r_i(y) \equiv \int_{-\infty}^{\infty} g_i(\sqrt{x^2+y^2})dx, \quad x = \frac{\xi_p}{2T},$$

$$r_i(0) = 1, \quad r_i(\infty) = 0, \quad i = a,b,c. \tag{23}$$

We define averaging over the Fermi surface

$$\langle f_p\rangle = \frac{\overline{f_p\delta(\xi_p)}}{\nu_F}, \quad \nu_F = \nu(E_F) = \overline{\delta(\xi_p)}, \tag{24}$$

where ν_F is the density of electron states per unit energy, volume, and spin at the Fermi level. In such a way we obtain

$$C_\nu(T) = \tfrac{2}{3}\pi^2 T \nu_F \langle r_c(y_p)\rangle \tag{25}$$

and

$$\frac{C_\Delta}{C_\nu} = \frac{12}{7\zeta(3)} \frac{\langle \chi_p^2 r_a(y_p)\rangle^2 \theta(T_c - T)}{\langle \chi_p^4 r_b(y_p)\rangle \langle r_c(y_p)\rangle}. \tag{26}$$

At T_c, where the gap is small and $r_i(0)=1$ this formula gives the Pokrovskii[1] result for the reduced specific heat jump

$$\frac{\Delta C}{C_N(T_c)} = \frac{12}{7\zeta(3)} \frac{\langle \chi_p^2\rangle^2}{\langle \chi_p^4\rangle}. \tag{27}$$

For the GL coefficient Eqs. (12) and (17), the approximation (22) gives

$$\alpha(\eta, T) = \frac{\nu_F}{T}\langle \chi_p^2 r_a(\Delta_p/2T)\rangle,$$

$$b(\eta, T) = \frac{7\zeta(3)\nu_F}{8\pi^2 T^2}\langle \chi_p^4 r_b(\Delta_p/2T)\rangle. \tag{28}$$

Then the specific heat takes the simple GL form for arbitrary temperatures

$$C(T) = C_\nu(\eta, T) + T\frac{\alpha^2(\eta, T)}{b(\eta, T)}\theta(T_c - T). \tag{29}$$

Here, for the functions on the right-hand side we have substituted the thermal equilibrium value of the order parameter $\eta(T) = |Q(T)|^2$, obtained from the solution of Eq. (8). This BCS formula (29) is an example how good the physical intuition was in the phenomenology of superconductivity. According to the Gorter-Casimir[9] model the specific heat is a sum of a "normal" part and another therm, governed by the temperature dependence of the order parameter and having exactly the GL form. The Gorter-Casimir two-fluid model has very simple physical grounds. In the self-consistent approximation, the entropy $S(T, \Delta(T))$ is a function of the temperature and a temperature-dependent order parameter $\Delta(T)$. The temperature differentiation $C(T) = T(dS/dT)$ inevitably gives two terms in Eq. (9). According to the general idea by Landau,[10] the order parameter is an adequate notion for description of second-order phase transitions, regardless of the concrete particle dynamics. The ϵ expansion by Wilson and Fisher is only an ingenious realization of the same Landau idea when the influence of fluctuations is essential.

Again, at T_c the general formulas Eq. (28) give the Gor'kov and Melik-Barkhudarov[2] result for the GL coefficients

$$\alpha(0, T_c) = \frac{\nu_F}{T_c}\langle \chi_p^2\rangle, \quad b(0, T_c) = \frac{7\zeta(3)\nu_F}{8\pi^2 T_c^2}\langle \chi_p^4\rangle. \tag{30}$$

This result can be directly derived[7] from the variational free energy $F(\eta, T)$ of the superconductor, which close to T_c has the GL form

$$F_{GL}(\eta, T) \approx \alpha(0, T_c)(T - T_c)|Q|^2 + \tfrac{1}{2}b(0, T_c)|Q|^4. \tag{31}$$

The simplest method to calculate the GL coefficients is to differentiate[7] the free energy after a u-v transformations $F(\eta, T) = \overline{H} - TS$. Then

$$\alpha(0, T_c) = (\partial_\eta F)_T(\eta = 0, T = T_c),$$

$$b(0, T_c) = (\partial_\eta^2 F)_T(\eta = 0, T = T_c). \tag{32}$$

If a Van Hove singularity (VHS) is close to the Fermi level, then the formulas for GL coefficients are slightly modified[8]

$$\alpha(0, T_c) = \frac{\langle \chi_p^2\rangle}{T_c}\int_{-\infty}^{+\infty} \nu(E_F + 2T_c x) g_a(x) dx,$$

$$b(0, T_c) = \frac{7\zeta(3)\langle \chi_p^4\rangle}{8\pi^2 T_c^2}\int_{-\infty}^{+\infty} \nu(E_F + 2T_c x) g_b(x) dx,$$

$$C_\nu(T_c) = \frac{2}{3}\pi^2 T_c \int_{-\infty}^{+\infty} \nu(E_F + 2T_c x) g_c(x) dx. \tag{33}$$

Some important references on the influence of the VHS on the properties of superconductors and pioneering works on the two-band model are given in Ref. 8. Let us evaluate the upper limit that can give a VHS. Let us take the one-dimensional (1D) density of states $\nu(E) \propto 1/\sqrt{E - E_{\mathrm{VHS}}}$ and $E_F = E_{\mathrm{VHS}} = 0$; there is no doubt that this mathematical illustration is unphysical. In this case we have for the reduced specific heat jump $\Delta C/C_N(T_c)$, Eq. (27), an additional factor

$$\frac{\left[\int_0^\infty g_a(\tilde{x}^2) d\tilde{x}\right]^2}{\int_0^\infty g_c(\tilde{x}^2) d\tilde{x} \int_0^\infty g_b(\tilde{x}^2) d\tilde{x}} = 2.51, \quad \tilde{x} \propto \sqrt{E}. \tag{34}$$

Although this mathematical example is not realistic, it can be seen that the VHS emulates qualitatively strong-coupling corrections to the BCS theory: an enhancement of $\Delta C/C_N(T_c)$ and $2\Delta_{\max}(0)/T_c$. Another simulation of strong-coupling effects can be demonstrated by a simple model density of states, corresponding to the case of layered cuprates

$$\nu(\xi) = 1 + k \ln \frac{1}{|\xi - E_{\mathrm{VHS}}|}. \tag{35}$$

For illustration, we solve the equation

$$\int_{-\omega_D}^{\omega_D} \frac{\tanh(\sqrt{\xi^2 + \Delta^2(T)}/2T)}{2\sqrt{\xi^2 + \Delta^2(T)}} \nu(\xi) d\xi = G^{-1} \tag{36}$$

taking $\omega_D = 10$, $G = 1/2$, and $k = 10$. The $Z \equiv [2\Delta(0)/T_c]/(2\pi/\gamma)$ versus E_{VHS}/T_c plot is given in Fig. 1. It can be seen that 7% enhancement corresponds to $E_{\mathrm{VHS}} = T_c$. Thus, the influence of the VHS on the specific heat is much stronger than on the $\Delta(0)/T_c$ ratio.

Let us also recall the general GL formula for the specific heat jump at T_c

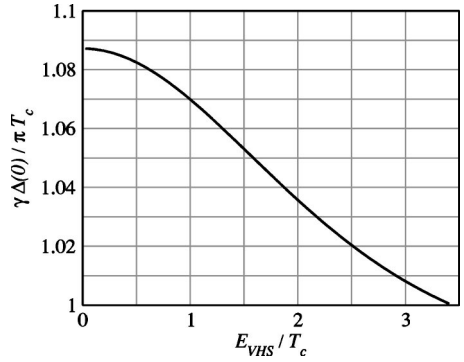

FIG. 1. $Z \equiv [2\Delta(0)/T_c]/(2\pi/\gamma)$ vs E_{VHS}/T_c computed for the model density of states Eq. (35). Note that 7% enhancement corresponds to $E_{\mathrm{VHS}}=T_c$ and the maximum enhancement is $\approx$9%.

$$\Delta C = T_c \frac{\alpha^2(0,T_c)}{b(0,T_c)}. \tag{37}$$

The two-band model provides probably the simplest possible illustration of the derived formula for the specific heat (for pioneering references on the two-band model see Ref. 8). The model is applicable with a remarkable accuracy[11] to MgB_2—a material that has been in the limelight in the physics of high-T_c superconductivity over past years.

For the normal specific heat we have

$$C_\nu(T) = \tfrac{2}{3}\pi^2 T \nu_F [c_1 r_c(y_1) + c_2 r_c(y_2)], \tag{38}$$

where

$$y_1 = \frac{\Delta_1}{2T}, \quad y_2 = \frac{\Delta_2}{2T}, \quad c_1 + c_2 = 1, \tag{39}$$

and $c_1\nu_F$ and $c_2\nu_F$ are the densities of states for the two bands of the superconductor. Above T_c or in the case of strong magnetic fields $B > B_{c2}$ we have

$$C_N(T) = \tfrac{2}{3}\pi^2 \nu_F T. \tag{40}$$

As pointed out earlier, within the weak-coupling BCS approximation, Pokrovskii[1] has proved the general separation of the variables [Eq. (5)] that for a two-band superconductor results in a weakly temperature-dependent gap ratio $\delta = \Delta_1/\Delta_2 = \chi_1/\chi_2$. For MgB_2 determination of the two gaps has been carried out by directional point-contact spectroscopy[12] in single crystals. One can see that for model evaluations the temperature dependence of the gap ratio could be neglected.

For the moments of the gap we have[13]

$$\left\langle \chi_p^n r_i\left(\frac{\Delta_p}{2T}\right)\right\rangle = \frac{c_1\delta^n r_i(y_1) + c_2 r_i(y_2)}{(c_1\delta^2 + c_2)^{n/2}}, \quad i = a,b,c \tag{41}$$

where the normalization is irrelevant in further substitution in the GL coefficients. Finally, for the second GL order-parameter term of the specific heat below the T_c we obtain

$$C_\Delta(T) = \frac{8\pi^2}{7\zeta(3)}\nu_F T \frac{[c_1\delta^2 r_a(y_1) + c_2 r_a(y_2)]^2}{c_1\delta^4 r_c(y_1) + c_2 r_c(y_2)}. \tag{42}$$

For the jump of the specific heat this formula reduces to the Moskalenko[14] result

$$\frac{\Delta C}{C_N(T_c)} = \frac{12}{7\zeta(3)} \frac{(c_1\chi_1^2 + c_2\chi_2^2)^2}{c_1\chi_1^4 + c_2\chi_2^4}, \tag{43}$$

which is, in fact, a special case of the Pokrovskii[1] formula [Eq. (27)] applied to the two-band model. For application of the two-band model to the specific heat of MgB_2, the reader is referred to Ref. 13.

The analysis of the specific heat for MgB_2 gives perhaps the best corroboration of the BCS results due to Pokrovskii[1] and Moskalenko.[14] Solving the Eliashberg equation and performing first-principle calculations for the specific heat of MgB_2, Golubov *et al.* (Ref. 15, Fig. 3) derived 65% reduction of the specific heat jump at T_c. On the other hand, Eqs. (27) and (43), using the parameters from Ref. 15, give $\langle\chi^2\rangle^2/\langle\chi^4\rangle = 58\%$ reduction of the $\Delta C/C_N(T_c)$ ratio. The 7% difference between those two estimates is in the range of the experimental accuracy, and the Eliashberg corrections to the BCS result is difficult to extract. Unfortunately, the groups solving the Eliashberg equation have not compared their results to the classical results of the BCS theory for anisotropic superconductors[1] in order to analyze several percent strong-coupling corrections to the specific heat jump for MgB_2.

In the single-band case $c_1 = 1$ and Eq. (42) gives a simple relation between the specific heat and the BCS isotropic gap

$$\frac{C(T)}{C_N(T)} = r_c(y) + \frac{12}{7\zeta(3)}\frac{r_a^2(y)}{r_b(y)}, \tag{44}$$

where $y(T) = \Delta(T)/2T$. For anisotropic superconductors, functions of the gap have to be averaged independently on the Fermi surface; this is the interpretation of the general formulas [Eq. (28) and Eq. (29)]. Thus, we have the natural generalization

$$\frac{C(T)}{C_N(T)} = \langle r_c(y_p)\rangle + \frac{12}{7\zeta(3)}\frac{\langle\chi_p^2 r_a(y_p)\rangle^2}{\langle\chi_p^4 r_b(y_p)\rangle}, \tag{45}$$

where $y_p(T) = \Delta_p(T)/2T = \chi_p Q(T)/2T$.

For illustration, we now apply this general formula to three typical cases and the results are shown in Fig. 2: (i) the isotropic-gap BCS model $\chi_p = 1$, familiar from a number of textbooks;[16–18] (ii) the two-dimensional (2D) *d*-wave superconductor $\chi_p = \cos 2\varphi$, $\tan\varphi = p_y/p_x$; and (iii) a two-band superconductor $c_1 = c_2 = 1/2$, for which the gap ratio parameter is taken to reproduce the same reduced specific heat jump of the *d*-wave superconductor ($\delta = \sqrt{3 \pm \sqrt{8}} = 2.41$ or 0.41).

The latter two models are often applied to analyze the behavior of CuO_2 or MgB_2 superconductors. Note also the qualitative difference. For a *d*-wave superconductor we have a quadratic specific heat at $T \ll T_c$, whereas for a two-band superconductor we have the exponential behavior $C(T) \propto \exp(-\Delta_2/2T)$ (see also Fig. 3).

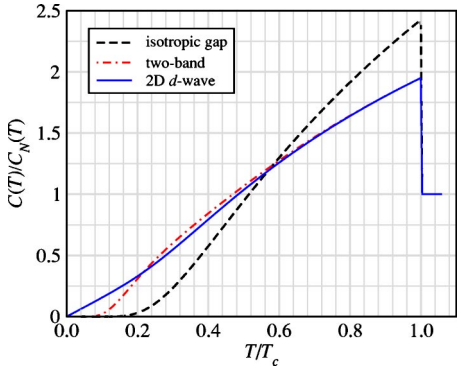

FIG. 2. (Color online) Superconducting-to-normal specific heat ratio $C(T)/C_N(T)$ vs the reduced-temperature $t=T/T_c$ according to Eq. (45) computed for (i) an isotropic-gap BCS superconductor (dashed line), (ii) a two-band superconductor $c_1=c_2=1/2$ with a gap ratio parameter $\delta=2.41$ (dash-dotted line), and (iii) the 2D d-wave superconductor $\chi_p=\cos 2\varphi$, $\tan\varphi=p_x/p_y$ (solid line). Note that for $t>0.2$ two of the curves would be experimentally indistinguishable.

Consider now the low-temperature behavior of the specific heat per unit area for a 2D d-wave superconductor. Close to a node, the gap is proportional to the momentum component along the Fermi contour $\Delta_p(0)\approx v_\Delta p_l$. The corresponding superfluid velocity v_Δ is much smaller than the Fermi velocity v_F, which parametrizes the dependence of the normal excitations energy $\xi_p\approx v_F p_t$ as a function of the transversal to the Fermi contour momentum component. For the groundstate quasiparticle spectrum we have $E_p\approx\sqrt{v_\Delta^2 p_l^2+v_F^2 p_t^2}$. It is convenient to introduce the dimensionless variables $q_1=v_\Delta p_l/2T$ and $q_2=v_F p_t/2T$. In terms of the latter we have for the area element in momentum space

$$4\frac{dp_l dp_t}{(2\pi\hbar)^2}=4\frac{(2T)^2}{v_\Delta v_F}\frac{2\pi q\,dq}{(2\pi\hbar)^2}=\frac{2EdE}{\pi\hbar^2 v_\Delta v_F}, \tag{46}$$

where $q=\sqrt{q_1^2+q_2^2}=z_p=E_p/2T$, and for axial symmetric functions we can use polar coordinates (cf. Ref. 19). Here we have taken into account four nodal points. In such a way Eq. (10) gives

$$C_\nu(T\ll T_c)=\frac{16}{\pi\hbar^2}\frac{T^2}{v_\Delta v_F}\int_0^\infty\frac{q^3dq}{\cosh^2 q}\approx 6.89\frac{T^2}{\hbar^2 v_\Delta v_F}, \tag{47}$$

where we have used $18\zeta(3)/\pi\approx 6.89$ [cf. Ref. 19, Eq. 2.9]. This result together with Eq. (40) gives for the superconducting-to-normal specific heat ratio

$$\frac{C_\nu}{C_N}(t\ll 1)=1.047\frac{T_c}{\hbar^2\nu_F v_\Delta v_F}t, \tag{48}$$

where $t=T/T_c$ is the reduced temperature. The penetration depth has a similar linear low-temperature behavior for d-wave superconductors.

Very often fluctuations of stoichiometry and crystal defects make the theory of homogeneous crystal inapplicable close to the critical region. Let $T_c(\mathbf{r})$ be a weakly fluctuating Gaussian field of the space vector $\mathbf{r}$. Hence, the simplest possible empirical model is to apply a Gaussian kernel to the theoretically calculated curve. Then for the heat capacity we have

$$C(t)=\int_{-\infty}^{+\infty}C_{\text{theor}}(t)\exp\left\{-\frac{(t-t')^2}{2(\Delta t)^2}\right\}\frac{dt'}{\Delta t\sqrt{2\pi}}. \tag{49}$$

The philosophy of applying the convolution technique to all theoretical curves with singularities was advocated in the book by Migdal.[20] Such an empirically smeared curve with $\Delta t=0.027$ describes better the experimental data for MgB_2 close to T_c; $T_c\Delta t\approx 1.1$ K, $B_{c2}(0)=2.5$ T, and $B_{c2}(0)\Delta t=750$ G. The result is depicted in Fig. 3, where the smeared theoretical curve is compared to the experimental data.[11] In order to achieve a good fit of the theory to the experimental data we have treated c_1 and δ as fitting parameters (cf. Refs. 11, 13, 21, and 22). The values used $c_1=0.49$ and $\delta=2.9$ are slightly different from the set of parameters used later for computing the penetration depth, but are still in agreement with different spectroscopic evaluations. In order to reach the analogous quality of the fit of $C(T)$ for cuprates we have to take into account simultaneously the gap anisotropy and the VHS in the general expressions [Eq. (12) and Eq. (17)].

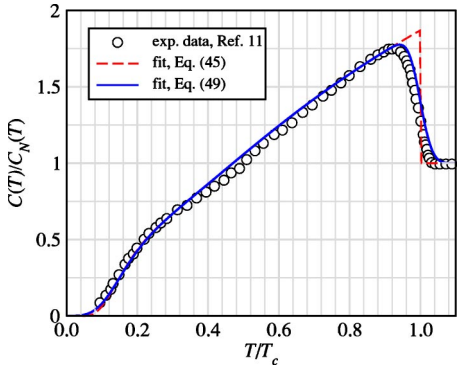

FIG. 3. (Color online) Comparison between the superconducting-to-normal specific heat ratio $C(T)/C_N(T)$; the theoretical curve is computed following Ref. 13 with $c_1=0.49$, $\delta=2.9$ (solid line) and the experimental data for MgB_2 are taken from Ref. 11 (circles). The theoretical curve is convoluted with a Gaussian kernel [Eq. (49)], chosen to fit best the experimental data ($\Delta t=0.027$). The experimental data[11] are digitized from Fig. 3 of Ref. 13.

An analogous to Eq. (49) smearing of the fluctuation magnetization above T_c reads

$$M(B,T-T_c)=\int M_{\text{theor}}(B,T-T_c')\exp\left\{-\frac{(T_c'-T_c)^2}{2(T_c\Delta t)^2}\right\}\times\frac{dT_c'}{\sqrt{2\pi}T_c\Delta t}. \tag{50}$$

However, for big fluctuations of T_c we have to take into account the appearance of superconducting domains. Such a precise investigation of fluctuations in the magnetization of Nb and Sn in the past led to the discovery of twinning-plane superconductivity. For analytical GL results for twinning-plane superconductivity see Ref. 23.

Here we wish to emphasize that a large body of experimental data for $B_{c2}(T)$ are strongly influenced by the disor-

der. It is imperative to cut off a region of width $T_c\Delta t$ or $B_{c2}(0)\Delta t$ close to $B_{c2}(T_c)$ if we wish to determine $B_{c2}(T)$ by extrapolation of properties from the superconducting phase or fluctuation behavior of the normal phase. Various spurious curvatures of $B_{c2}(T)$ have been reported merely as a result of disorder of the crystals.

II. ELECTRODYNAMIC BEHAVIOR

An analysis of the London penetration-depth tensor, similar to that carried out by Kogan in Ref. 3, gives

$$[\lambda^{-2}(T)]_{\alpha\beta} = \frac{e^2}{\varepsilon_0 c^2} 2\nu_F \langle r_d(y_p) v_\alpha v_\beta \rangle, \quad \alpha,\beta = x,y,z, \quad (51)$$

where

$$\mathbf{v}_p = \frac{\partial \varepsilon_p}{\partial \mathbf{p}}, \quad m_p^{-1} = \frac{\partial \mathbf{v}_p}{\partial \mathbf{p}} = \frac{\partial^2 \varepsilon_p}{\partial \mathbf{p}^2} \quad (52)$$

are the band velocity and effective mass and

$$r_d(y) \equiv (y/\pi)^2 \sum_{n=0}^{\infty} \left[(y/\pi)^2 + \left(n + \frac{1}{2} \right)^2 \right]^{-3/2}, \quad (53)$$

$$r_d(y) \approx 7\zeta(3)(y/\pi)^2 \ll 1, \quad r_d(\infty) = 1.$$

For comparison, the conductivity tensor of the normal phase in the τ_p approximation reads

$$\sigma_{\alpha\beta} = 2\nu_F e^2 \langle \tau_p v_\alpha v_\beta \rangle. \quad (54)$$

For penetration depths along the principal crystal axes we have in the two-band model

$$\lambda_\alpha^{-2}(T) = \lambda_{\alpha,1}^{-2}(0) r_d(y_1) + \lambda_{\alpha,2}^{-2}(0) r_d(y_2), \quad (55)$$

where for uniaxial crystals, such as MgB_2, there are only four constants: $\lambda_{x,1}(0) = \lambda_{y,1}(0)$, $\lambda_{x,2}(0) = \lambda_{y,2}(0)$, $\lambda_{z,1}(0)$, and $\lambda_{z,2}(0)$. These can be obtained from electron-band calculations,[24]

$$[\lambda^{-2}(T)]_{\alpha\beta} = \frac{e^2}{\varepsilon_0 c^2} 2\nu_F \sum_{b=1,2} c_b r_d\left(\frac{\Delta_b(T)}{2T} \right) \langle v_\alpha v_\beta \rangle_b = \sum_{b=1,2} (\lambda_b^{-2}(0))_{\alpha\beta} r_d\left(\frac{\Delta_b(T)}{2T} \right), \quad (56)$$

where the band index b labels the leaf of the Fermi surface over which the averaging of the electron velocities is carried out. For a discussion and details see the review by Kogan and Bud'ko.[3] There is a natural "Eliashbergization" of this result (cf. Refs. 15, 22, and 25–27):

$$r_d\left(\frac{\Delta_p}{2T} \right) = \sum_{n=0}^{\infty} \frac{2\pi T \Delta_p^2}{(\Delta_p^2 + \omega_n^2)^{3/2}} \to \sum_{n=0}^{\infty} \frac{2\pi T \tilde{\Delta}_p^2}{[\tilde{\Delta}_p^2(\omega_n) + \tilde{\omega}_{n,p}^2]^{3/2}}, \quad (57)$$

where $\omega_n = (2n+1)\pi T$ are the Matsubara frequencies, $\tilde{\omega}_{n,p} = Z_p(\omega_n)\omega_n$, $\tilde{\Delta}_p(\omega_n) = Z_p(\omega_n)\Delta_p(\omega_n)$ and $Z_p(\omega_n)$ is the normalization factor. Analogous expressions can be worked out for the specific heat.

For a heuristic consideration of the result by Kogan[3] at $T=0$ see Ref. 24. At $T=0$ the Fermi surface is shifted as a rigid object in the momentum space under the influence of the electromagnetic field. This shift of all conduction electrons explains why for the penetration depth the influence of VHS is less essential than the influence on the heat capacity. The increase of the kinetic energy of all conduction electrons is actually the increase of the Gibbs free-energy density $\Delta G = (1/2\varepsilon_0 c^2)\lambda^2 j^2$. At finite temperatures the number of superfluid electrons is $r_d(\Delta_p/2T)$ times smaller.

The penetration depths at $T=0$ can be also expressed by the optical masses and the Hall constant of the normal metal at high magnetic field

$$[\lambda^{-2}(0)]_{\alpha\beta} = \frac{e}{\varepsilon_0 c^2} \frac{1}{\mathcal{R}_\infty} (m^{-1})_{\alpha\beta},$$

$$\frac{1}{\mathcal{R}_\infty} = 2e \int_{\varepsilon_p < E_F} \frac{d^3p}{(2\pi\hbar)^3},$$

$$m^{-1} = \frac{\int_{\varepsilon_p < E_F} \frac{d^3p}{(2\pi\hbar)^3} m_p^{-1}}{\int_{\varepsilon_p < E_F} \frac{d^3p}{(2\pi\hbar)^3}} = \frac{\oint_{\varepsilon_p = E_F} \frac{dS_p}{(2\pi\hbar)^3 v_p} \mathbf{v}_p \otimes \mathbf{v}_p}{\int_{\varepsilon_p < E_F} \frac{d^3p}{(2\pi\hbar)^3}}, \quad (58)$$

the last equation being a consequence of the Gauss theorem $\int_{\varepsilon_p < E_F} d^3p (\partial/\partial \mathbf{p}) = \oint_{\varepsilon_p = E_F} d\mathbf{S}_p$, where $d\mathbf{S}_p$ is the element of the Fermi surface oriented along the outward normal. For an extensive discussion on galvanomagnetic properties of normal metals and inclusion of hole pockets with volume density n_h for $\mathcal{R}_\infty^{-1} = e(n_e - n_h)$ see the textbook by Lifshitz and Pitaevskii[28] or the monograph by Lifshitz, Azbel, and Kaganov.[29] The Bernoulli effect can be easily observed in almost compensated superconductors for which $n_e \approx n_h$ and the Hall constant is bigger.

In the superconducting phase the Hall constant $\mathcal{R}_\infty$ can be determined by the Bernoulli potential

$$\Delta\varphi = -\mathcal{R}_\infty \frac{1}{2\varepsilon_0 c^2} \lambda^2(T) j^2; \quad (59)$$

generalization for the anisotropic case can be obtained by the obvious replacement $\lambda^2 j^2 \to j_\alpha \lambda_{\alpha\beta}^2 j_\beta$. Here we suppose that $j \ll j_c(T)$, j_c being the critical current. If the magnetic field $\mathbf{B}$ is parallel to the surface of a bulk superconductor this formula gives

$$\Delta\varphi = -\mathcal{R}_\infty \frac{B^2}{2\mu_0}. \quad (60)$$

All charge carriers interact with the electric potential φ, but only the superfluid part $\propto r_d(\Delta_p/2T)$ creates kinetic energy. The constancy of the electrochemical potential in the superconductor gives the change of the electric potential, i.e., the Bernoulli effect. For the temperature-dependent condensation energy $\Delta G = -B_c^2(T)/2\mu_0$ the corresponding change of the electric potential is given by

$$\Delta\varphi = \mathcal{R}_\infty \frac{B_c^2(T)}{2\mu_0}. \tag{61}$$

For complete determination of the Hall constant $\mathcal{R}_\infty$, the penetration depth $\lambda(T)$, and the optical mass of conduction electrons in a clean superconductor [cf. Ref. 24, Eq. (20)],

$$m = \frac{e\lambda^2(0)}{\varepsilon_0 c^2 \mathcal{R}_\infty}, \tag{62}$$

we have to investigate the Bernoulli effect for thin, $d_{\text{film}} \ll \lambda(T)$, and thick, $d_{\text{film}} \gg \lambda(T)$, superconducting films of the same material. $M_{\text{cp}} \equiv 2m$ can be called effective mass of the Cooper pairs; this parameter can be significantly increased by disorder.

For the temperature dependence of the electrochemical potential of the normal phase we have [Ref. 29, Eq. (12.16)]

$$e\Delta\varphi = \frac{\pi^2}{6}\frac{\nu'(E_F)}{\nu(E_F)}T^2. \tag{63}$$

Close to a VHS the influence of the energy derivative of the density of states can be significant and measurable.

The entropy and specific heat related to the volume density of the free energy of superconducting condensation $B_c^2(T)/2\mu_0$ can be determined by electric capacitor measurements, applying surface-temperature oscillations. For discussions of possible experimental setups see Ref. 24 and references therein.

It is a matter of technical calculations to verify the identity

$$(y/\pi)^2 \sum_{n=0}^{\infty} \left[(y/\pi)^2 + \left(n+\frac{1}{2}\right)^2 \right]^{-3/2} + \int_{-\infty}^{+\infty} \frac{dx}{2\cosh^2\sqrt{x^2+y^2}} = 1, \tag{64}$$

which transcribes into the form

$$r_a(y) + r_d(y) = 1. \tag{65}$$

In such a way the *electrodynamic behavior* of a superconductor can be expressed in terms of the functions, defined for description of its *thermodynamic behavior*. Using Eqs. (65) and (51) we obtain

$$\rho_N(T) = 1 - \frac{[\lambda^{-2}(T)]_{\alpha\beta}}{[\lambda^{-2}(0)]_{\alpha\beta}} = \frac{\left\langle r_a\left(\frac{\Delta_p}{2T}\right) v_\alpha v_\beta \right\rangle}{\langle v_\alpha v_\beta \rangle}. \tag{66}$$

Within the framework of London electrodynamics, $\rho_N(T) = 1 - \lambda^2(0)/\lambda^2(T)$ is the normal fluid density and $\rho_S(T) = \lambda^2(0)/\lambda^2(T)$ is the superfluid one, having total charge density $\rho_S(T)/\mathcal{R}_\infty$. For a two-band superconductor, Eqs. (56) and (66) give for the penetration depth along the principal crystal axes

$$\rho_S(T) = \frac{\lambda_\alpha^2(0)}{\lambda_\alpha^2(T)} = \sum_{b=1,2} w_{\alpha,b} r_d \frac{\Delta_b(T)}{2T}, \quad w_{\alpha,b} = c_b \frac{\langle v_\alpha^2 \rangle_b}{\langle v_\alpha^2 \rangle},$$

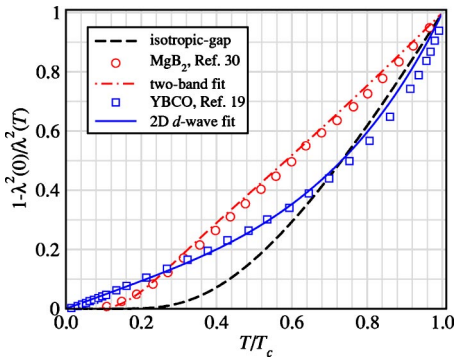

FIG. 4. (Color online) In-plane normal fluid density $1-\lambda^2(0)/\lambda^2(T)$ vs reduced temperature $t=T/T_c$ computed for three cases: (i) isotropic-gap BCS superconductor (dashed line), (ii) two-band superconductor MgB_2 with parameters $c_1=0.59$, $\delta=7.1/2.8$ (dash-dotted line), and (iii) 2D d-wave superconductor (solid line). The experimental points for $YBa_2Cu_3O_{7-\delta}$ (squares) are digitized from Ref. 19, and the corresponding theoretical 2D d-wave curve is calculated according to Eq. (68) with the renormalization factor $Z=1.4$. Some experimental points for MgB_2 (circles) are digitized from Fig. 9 of Ref. 30 (for details see the original work).

$$w_{\alpha,1} + w_{\alpha,2} = 1, \quad \langle v_\alpha^2 \rangle = c_1 \langle v_\alpha^2 \rangle_1 + c_2 \langle v_\alpha^2 \rangle_2. \tag{67}$$

For a set of parameters see the review by Kogan and Bud'ko.[3] We take $\delta=7.1/2.8$ according to the spectroscopic data[13,31] (see also the point contact spectroscopy data in Ref. 32). In Fig. 4 we compare our theoretical calculation with the experimental data for $\lambda(T)$ by Carrington and Manzano.[30] Here we take $c_1=0.59$, which gives $w_{a,1} \approx w_{a,2} \approx 0.5$. The functions $r_i(y)$ for $i=a,b,c,d$ can be easily programmed for the purposes of experimental data processing. The graphs of $r_i(y)$ and the corresponding $g_i(z)$ functions are given in Figs. 5 and 6. The temperature dependence of the penetration depth $\lambda(T)$ is also programmed for isotropic-gap, two-band, and model 2D d-wave superconductors. In the 2D d-wave case the theoretical result is compared to the experimental data[19] for $YBa_2Cu_3O_{7-\delta}$, which is also depicted in Fig. 4. The linear dependence of $1-\lambda^2(0)/\lambda^2(T)$ at low temperatures for $YBa_2Cu_3O_{7-\delta}$ is discussed in Eq. (2.10) of Ref. 19. For a 2D d-wave superconductor the general formula [Eq. (51)] gives

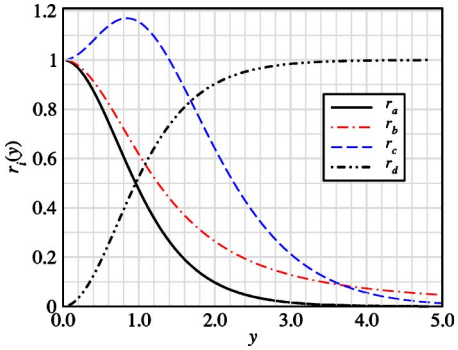

FIG. 5. (Color online) Plot of the $r_i(y)$ functions $(i=a,b,c,d)$.

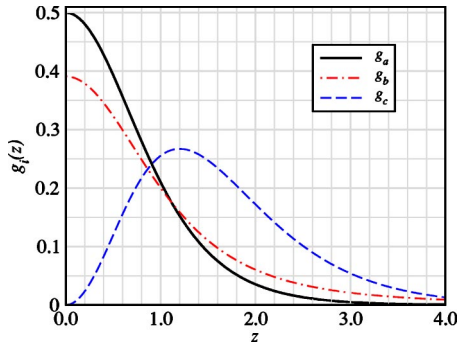

FIG. 6. (Color online) Plot of the $g_i(z)$ functions $(i=a,b,c)$.

$$\rho_S(T) = \frac{\lambda^2(0)}{\lambda^2(T)} = \int_0^{2\pi} r_d\left(Z\frac{\Delta_{\max}(T)}{2T}\cos 2\varphi\right)\frac{d\varphi}{2\pi}, \quad (68)$$

where the temperature dependence of the order parameter is described in the Appendix. We are using an oversimplified model for cuprate superconductivity for which are neglected (i) the anisotropy of the Fermi velocity $v_F(\mathbf{p})$ along the Fermi contour, (ii) higher harmonics of the gap function Δ_p along the Fermi contour, and (iii) the influence of VHS of the density of states slightly below the Fermi level. For comparison between angle resolved photoemission spectroscopy (ARPES) data and a lattice model for high-T_c spectrum see Fig. 3 of Ref. 4.

Let us assume now that the order parameter for $YBa_2Cu_3O_{7-\delta}$ is Z times higher than the BCS prediction. This could be due to the influence of VHS or, which is more important, strong coupling effects. Inserting here $Z=1.4$ we can see that such a renormalization well describes the temperature dependence of the penetration depth in the whole temperature interval. Finally, we have a good working BCS-like formula. In fact, significantly higher $\Delta_{\max}(0)/T_c$ than BCS prediction is in agreement with the ARPES data.

III. THE CASE FOR Sr_2RuO_4

Our approach is also applicable to the triplet superconductor Sr_2RuO_4 (for a review, see Ref. 33). We adopt the promising gap anisotropy model by Zhitomirsky and Rice,[34] which gives $E_p=\sqrt{\xi_p^2+|\Delta_p|^2}$, with

$$|\Delta_p|^2 \propto \left[\sin^2\frac{p_x a}{2\hbar}\cos^2\frac{p_y a}{2\hbar} + \cos^2\frac{p_x a}{2\hbar}\sin^2\frac{p_y a}{2\hbar}\right]\cos^2\frac{p_z c}{2\hbar}, \quad (69)$$

where $p_x a/\hbar$, $p_y a/\hbar$, $p_z c/\hbar \in (0,2\pi)$. For the Fermi surface we take a simple cylinder $\varepsilon_p \approx \varepsilon(\sqrt{p_x^2+p_y^2})$ with radius $p_F a/\hbar \approx 0.93\ \pi$. Our calculations are depicted in Fig. 7. In this model calculation we have taken into account only one band responsible for superconductivity. Although it is not *a priori* clear how "good" this assumption is, our curve reproduces the theoretical curve by Zhitomirsky and Rice[34] and passes close to the experimental points by NishiZaki *et al.*[35] This promising success encouraged us to present the theoretical prediction for the penetration depth calculated from Eq. (66). According to the conclusions by Zhitomirsky and Rice,[34] their model with horizontal line nodes (see also Ref. 36) describes the experimental data better than a model with vertical line nodes. For illustration, in Fig. 7 we present also our calculations for a simple 2D vertical line nodes model with gap anisotropy function

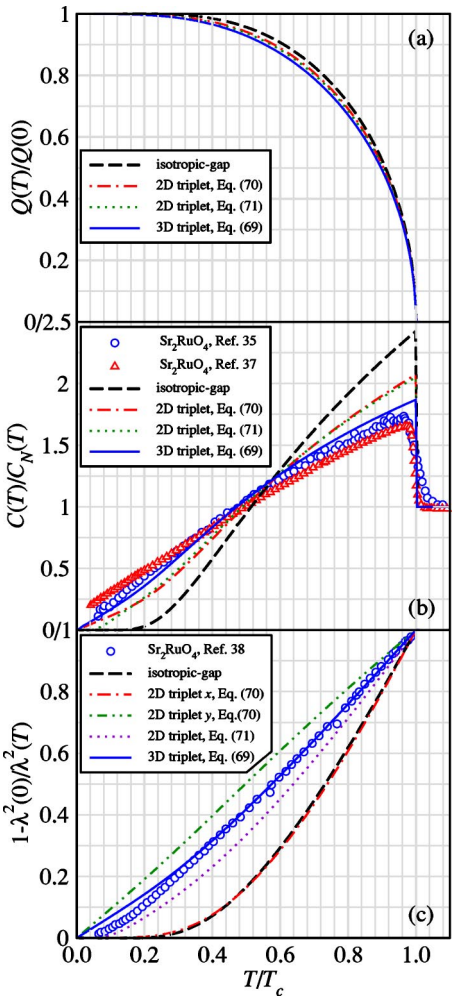

FIG. 7. (Color online) Sr_2RuO_4. (a) Reduced order parameter for the Zhitomirsky and Rice model [Eq. (69)] (solid line), the 2D vertical line nodes model [Eq. (70)] (dot-dashed line), and for the 2D model by Deguchi *et al.* [Eq. (71)] (dotted line). (b) Specific heat ratio $C(T)/C_N(T)$ for the Zhitomirsky and Rice model (solid line), the 2D vertical line nodes model (dash-dotted line), and for the Deguchi *et al.* model (dotted line). The experimental points (circles) from Ref. 35 are digitized from Fig. 1 of Ref. 34. (c) Normal fluid density $1-\lambda^2(0)/\lambda^2(T)$ corresponding to the gap anisotropy models (69)–(71). The experimental points (circles) from Ref. 38 are digitized from Fig. 2 of Ref. 39. We should note that the model with vertical line nodes predicts spontaneous breaking of the symmetry of the penetration depth in the *ab* plane.

$$\chi_p \propto \sin\left(\frac{p_x a}{2\hbar}\right). \quad (70)$$

Similar model was studied by NishiZaki *et al.*[35] (see also Fig. 26 in the review by Mackenzie and Maeno).[33]

From an aesthetic point of view our preferences are for the recent model for the gap anisotropy by Deguchi *et al.*[37]

$$|\Delta_p|^2 \propto \sin^2(p_x a/\hbar) + \sin^2(p_y a/\hbar). \quad (71)$$

Such types of anisotropy can be derived in the framework of quasi-two-dimensional exchange models for perovskite superconductivity of the type of the considered for CuO_2 plane in Ref. 4. The theoretical prediction corresponding to Eq. (71) is also illustrated in Fig. 7 together with the experimental data by Deguchi *et al.*[37]

IV. DISCUSSION AND CONCLUSIONS

Let us discuss now the specific heat. We have shown that for factorizable kernels[5] the specific heat can be represented as a sum of a "normal" component $C_\nu(T)$ and a term dependent on the order parameter $C_\Delta(T)$, which has the same form as in the GL theory. There is one detail that is worth focusing on: for the *s*-*d* model for high-T_c superconductivity[4] the kernel is indeed separable because the contact interaction is localized in a single atom in the lattice unit cell. One should only substitute the spectrum of the superconductor at $T < T_c$ in the known expression for the GL coefficients from classical work of Gor'kov and Melik-Barkhudarov.[2] The final expression for the specific heat is a generalization of the result of Pokrovskii.[1] The derived formulas can be easily programmed for fitting the experimental data of anisotropic superconductors. For the jump of the specific heat at the critical temperature $\Delta C|_{T_c} = C_\Delta(T_c^-)$ general consideration has already been given in Ref. 7. The derived formula is not exact, but interpolates between the correct low-temperature behavior and the result by Pokrovskii[1] for the specific heat jump at T_c. That is why we believe that our interpolation formula [Eq. (29)] can be useful for preliminary analysis of the experimental data for the specific heat in superconductors; for experimental data processing the accuracy could be comparable (e.g., with the accuracy of the Debye formula for the phonon heat capacity).

We illustrated our formulas for $C(T)$ and $\lambda(T)$ for the isotropic-gap BCS model and three of the best investigated anisotropic-gap superconductors $YBa_2Cu_3O_{7-\delta}$, Sr_2RuO_4, and MgB_2. The nature of superconductivity for those superconductors is completely different: high-T_c and low-T_c, phonon- and exchange-mediated, singlet and triplet Cooper pairs. In all those cases the derived formulas work with an acceptable accuracy; in some cases we even have quantitative agreement and for high-T_c cuprates we have shown what the BCS analysis can give. We conclude that the statistical properties of the superconductors [thermodynamic $C(T)$ and kinetic $\lambda(T)$] are determined mainly by the gap anisotropy, irrespective of the underlying pairing mechanism, and the approximative weak coupling separation of variables[1] $\Delta_p(T) = Q(T)\chi_p$ is an adequate approach. It is worth applying the derived formulas for $C(T)$ and $\lambda(T)$ for every new superconductor. Often after the synthesis of a new superconductor, single crystals are not available and only the data for heat capacity $C(T)$ can help the theory to distinguish between different models for the gap anisotropy even before detailed spectroscopic investigation is performed.

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APPENDIX: ORDER PARAMETER EQUATION FOR ANISOTROPIC-GAP SUPERCONDUCTORS

Following Ref. 1, let us scrutinize the derivation of and the solution to Eq. (8). The gap anisotropy function will have nonzero values only in a narrow region near the Fermi surface

$$\chi_p = \chi_p \theta(\omega_D - |\xi_p|), \quad T_c \ll \omega_D \ll E_F. \quad (A1)$$

Later, the differential volume in the momentum space can be separated to Fermi surface element dS and a normal element dp_t

$$d^D p = dp_t dS = \frac{d\varepsilon}{v_F} dS, \quad v_F(\mathbf{p}) = \left| \frac{\partial \varepsilon_p}{\partial \mathbf{p}} \right|. \quad (A2)$$

Returning to Eq. (8) we have

$$\frac{G}{(2\pi\hbar)^D} \oint \int \frac{\chi_p^2}{2E_p} \tanh(z_p)\theta(\omega_D - |\xi_p|) \frac{d\varepsilon dS}{v_F} = 1, \quad (A3)$$

where $\oint$ denotes integration over the Fermi surface. With the account of the energy cutoff ω_D the latter reads

$$\frac{G}{(2\pi\hbar)^D} \oint \frac{dS}{v_F} \chi_p^2 \int_0^{\omega_D} \frac{\tanh(\sqrt{\xi^2 + \Delta_p^2}/2T)}{\sqrt{\xi^2 + \Delta_p^2}} d\xi = 1. \quad (A4)$$

According to Eq. (24) we have for the density of states

$$\nu_F = \overline{\delta(\xi_p)} = \frac{1}{(2\pi\hbar)^D} \int \delta(\varepsilon - E_F) d\varepsilon \frac{dS}{v_F} = \frac{1}{(2\pi\hbar)^D} \oint \frac{dS}{v_F}. \quad (A5)$$

Similarly, the averaging over the Fermi surface can be represented as a surface integral

$$\langle f(p) \rangle = \frac{1}{\nu_F} \oint \frac{dS}{(2\pi\hbar)^D v_F} f(p). \quad (A6)$$

In these notation Eq. (A4) reads

$$\left\langle \chi_p^2 \int_0^{\omega_D} \frac{\tanh(\sqrt{\xi^2 + \Delta_p^2}/2T)}{\sqrt{\xi^2 + \Delta_p^2}} d\xi \right\rangle = \frac{1}{G\nu_F} = \frac{1}{\lambda_{\mathrm{BCS}}}, \quad (A7)$$

where $\lambda_{\mathrm{BCS}} \equiv G\nu_F$ is the dimensionless BCS coupling constant.

At $T = T_c$, where $\Delta_p = 0$ and $E_p = |\xi_p|$, substituting $x = \xi/2T$ we obtain

$$\langle \chi_p^2 \rangle \int_0^M \frac{\tanh x}{x} dx = \frac{1}{\lambda_{\mathrm{BCS}}}, \quad M = \frac{\omega_D}{2T_c} \gg 1. \tag{A8}$$

Now the identity

$$\int_0^M \frac{\tanh x}{x} dx = \ln\left(\frac{4\gamma}{\pi} M\right) \tag{A9}$$

gives

$$T_c = 2\omega_D \frac{\gamma}{\pi} \exp\left(-\frac{1}{\langle \chi_p^2 \rangle \lambda_{\mathrm{BCS}}}\right). \tag{A10}$$

Analogously, at $T=0$ we have

$$\left\langle \chi_p^2 \int_0^{\omega_D} \frac{d\xi}{\sqrt{\xi^2 + \Delta_p^2(0)}} \right\rangle = \frac{1}{\lambda_{\mathrm{BCS}}}. \tag{A11}$$

Then taking into account that $\omega_D \gg \Delta_p(0)$ we have

$$\int_0^{\omega_D} \frac{d\xi}{\sqrt{\xi^2 + \Delta_p^2}} = \ln\left(\frac{\omega_D}{|\Delta_p|} + \sqrt{1 + \frac{\omega_D^2}{|\Delta_p|^2}}\right) \approx \ln \frac{2\omega_D}{|\Delta_p|}. \tag{A12}$$

As we will see later, it is convenient to modify the normalization of the order parameter and gap anisotropy function

$$\tilde{\chi}_p = \frac{\chi_p}{\chi_{\mathrm{av}}}, \quad \tilde{Q} = Q\chi_{\mathrm{av}}, \quad \chi_{\mathrm{av}} \equiv \exp\left\{\frac{\langle \chi_p^2 \ln|\chi_p|\rangle}{\langle \chi_p^2 \rangle}\right\}. \tag{A13}$$

The renormalizing multiplier χ_{av} is chosen in order for the renormalized gap anisotropy function to obey the relation

$$\langle \tilde{\chi}_p^2 \ln \tilde{\chi}_p^2 \rangle = 0. \tag{A14}$$

For the two-band model this gives

$$\chi_{\mathrm{av}} = \chi_1^{c_1\chi_1^2} \chi_2^{c_2\chi_2^2}, \tag{A15}$$

and one can easily verify that

$$c_1 \tilde{\chi}_1^2 \ln|\tilde{\chi}_1| + c_2 \tilde{\chi}_2^2 \ln|\tilde{\chi}_2| = 0. \tag{A16}$$

Similarly, using

$$\int_0^{\pi/2} \cos^2 \varphi \ln|\cos \varphi| d\varphi = \frac{\pi}{8} \ln(e/4) \tag{A17}$$

we obtain for a 2D *d*-wave superconductor

$$\tilde{\chi}_p(\varphi) = \frac{2}{\sqrt{e}} \cos 2\varphi,$$

$$\int_0^{2\pi} \tilde{\chi}_p^2(\varphi) \ln|\tilde{\chi}_p(\varphi)| d\varphi = 0. \tag{A18}$$

Using the approximation (A12) with a renormalized order parameter and gap anisotropy function, from Eq. (A11) we derive

$$\tilde{Q}(0) = 2\omega_D \exp\left(-\frac{1}{\langle \chi_p^2 \rangle \lambda_{\mathrm{BCS}}}\right). \tag{A19}$$

This equation together with (A10) gives the well-known BCS relation for the renormalized order parameter for anisotropic superconductors[1]

$$\frac{2\tilde{Q}(0)}{T_c} = \frac{2\pi}{\gamma} \approx 3.53. \tag{A20}$$

We assume that the density of states $\nu(E)$ is almost constant in the energy interval $E_F \pm 2T_c$.

The renormalization does not change the gap $\Delta_p(T) = Q\chi_p = \tilde{Q}\tilde{\chi}_p$, but in a sense $\tilde{Q}(T)$ is the "true" BCS gap for an anisotropic superconductor. For $T=0$ the BCS model gives for *d*-wave superconductors $\Delta_p(0) = \Delta_{\max} \cos 2\varphi$, where

$$\frac{2\Delta_{\max}}{T_c} = \frac{2\pi}{\gamma} \frac{2}{\sqrt{e}} \approx 4.28. \tag{A21}$$

However, for cuprates we have to take into account the influence of Van Hove singularity and strong coupling correlations. As we fitted from the temperature dependence of the penetration depth for $YBa_2Cu_3O_{7-\delta}$, we have 40% bigger gap $\Delta_{\max} = Z\Delta_{\max}^{(\mathrm{BCS})}$ and $2\Delta_{\max}/T_c \approx 6.0$. In such a way the thermodynamic behavior is in agreement with the spectroscopic data. This is a good hint in favor of the Landau-Bogoliubov quasiparticle picture applied to high-T_c cuprates. For MgB_2 taking $c_1 = 0.44$ and $\Delta_1(0) = 7.1$ meV and $\Delta_2(0) = 2.8$ we obtain $\tilde{\chi}_1 \approx 1.17$ and $\tilde{\chi}_2 \approx 0.46$. Then $\tilde{Q}(0) = \Delta_1(0)/\tilde{\chi}_1 = \Delta_2(0)/\tilde{\chi}_2 \approx 6.08$ meV $= 70.6$ K. For the critical temperature $T_c = 39$ K we obtain $2\tilde{Q}(0)/T_c \approx 3.62$, which agrees with the BCS ratio (A20) within 3% accuracy as found in Ref. 13

For arbitrary temperatures using the identity

$$\tanh \frac{x}{2} = 1 - \frac{2}{e^x + 1}, \tag{A22}$$

Eq. (A7) reads

$$\left\langle \chi_p^2 \int_0^{\omega_D} \frac{d\xi}{\sqrt{\xi^2 + \Delta_p^2(T)}} \right\rangle - \frac{1}{\lambda_{\mathrm{BCS}}} = 2\left\langle \chi_p^2 \int_0^{\omega_D} \frac{d\xi}{\sqrt{\xi^2 + \Delta_p^2(T)} \left[\exp\left(\frac{\sqrt{\xi^2 + \Delta_p^2(T)}}{T}\right) + 1\right]} \right\rangle. \tag{A23}$$

Substituting here $1/\lambda_{\mathrm{BCS}}$ from Eq. (A11) and taking into account the $\omega_D \gg |\Delta_p(0)|$ approximation, [Eq. (A12)], we obtain the Pokrovskii equation

$$q := \exp\left\{-\frac{\langle \chi_p^2 F(2y_p)\rangle}{\langle \chi_p^2 \rangle}\right\}, \quad 2y_p = \frac{\pi}{\gamma} \frac{\chi_p}{\chi_{\mathrm{av}}} \frac{q}{t} = \frac{\Delta_p}{T}, \tag{A24}$$

where

$$q(t) = \frac{\Delta_p(T)}{\Delta_p(0)} = \frac{Q(T)}{Q(0)} = \frac{\tilde{Q}(T)}{\tilde{Q}(0)} \tag{A25}$$

is the reduced order parameter $0 \leqslant q \leqslant 1$ as a function of the reduced temperature $t = T/T_c$. In physical variables Pokrovskii[1] equation reads

$$\ln \frac{\Delta_p(T)}{\Delta_p(0)} + \langle \chi_p^2 F(\Delta_p(T)/T) \rangle_p = 0. \tag{A26}$$

The function $F(x)$ associated with the right-hand side of Eq. (A23) is defined by an integral, for which we have one integral and two different summation formulas, convenient for small and large arguments[40]

$$\begin{aligned} F(x) &\equiv \int_{-\infty}^{\infty} \frac{du}{\sqrt{u^2+x^2}[\exp(\sqrt{u^2+x^2})+1]} \\ &= 2\int_0^{\infty} \frac{du}{\exp(x\cosh u)+1} \\ &= \ln\frac{\pi}{\gamma x} + 2\pi\sum_{l=1}^{\infty}\left[\frac{1}{(2l-1)\pi} - \frac{1}{\sqrt{x^2+(2l-1)^2\pi^2}}\right] \\ &= -2\sum_{n=1}^{\infty}(-1)^n K_0(nx), \end{aligned} \tag{A27}$$

where for large arguments we have the approximate formula

$$2K_0(x \gg 1) \approx \sqrt{\frac{2\pi}{x}} e^{-x}\left(1 - \frac{1}{8x} + \frac{9}{128x^2} - \frac{225}{3972x^3}\right). \tag{A28}$$

Physically, here $x = \Delta/T$, $u = \xi/T$ and the upper integration bound ω_D/T has been replaced by ∞. For this function we have the approximate formulas

$$F(x \ll 1) \approx \ln\frac{\pi}{\gamma x} + \frac{7}{8\pi^2}\zeta(3)x^2, \tag{A29}$$

$$F(x \gg 1) \approx 2K_0(x). \tag{A30}$$

The Euler constant is $\gamma = e^C \approx 1.781\,072\,418$ and $\zeta(3) \approx 1.202\,056\,903$, where ζ is the Riemann zeta function. A plot of the function $F(x)$ is shown in Fig. 8. In the preprint version of this paper[41] a simple C++ code for numerical evaluation of $F(x)$ is provided. For fast calculations one has to take only several terms of the expansions [Eq. (A27)]. The $:=$ sign in Eq. (A24) represents an iterative assignment in which we use the initial approximation $q = 1$.

The BCS order-parameter equation (A24) is not specific for the physics of superconductivity. Recently, Abrikisov[42] has derived the same equation for the temperature dependence of the amplitude of spin density waves in cuprates.

For 2D d-wave superconductors the Pokrovskii equation (A24) reads

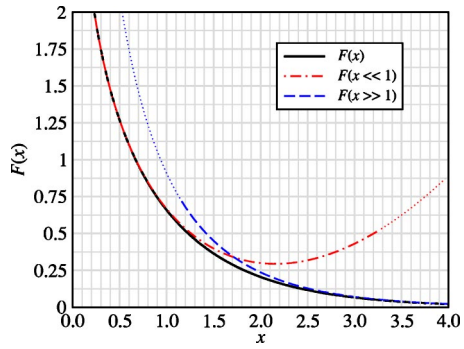

FIG. 8. (Color online) Plot of the $F(x)$ function. The approximations to $F(x)$ for $x \ll 1$ and $x \gg 1$ are given by Eqs. (A29) and (A30), respectively.

$$\ln q = -\int_0^{2\pi} 2\cos^2(2\varphi) F\left(\frac{2\pi}{\gamma\sqrt{e}}\cos(2\varphi)\frac{q}{t}\right)\frac{d\varphi}{2\pi}. \tag{A31}$$

The numerical solution for the squared reduced order parameter $q^2(t)$ is shown in Fig. 9. The linear dependence near the critical temperature $t = 1$ corresponds to the GL approximation. In Fig. 10 the squared reduced order parameter for MgB_2 (two-band model with $c_1 = 0.44$, $\delta = 7.1/2.8$) is compared to the experimental data from Ref. 31.

As a last problem, let us derive the factorizable kernel (7) as a result from the BCS equation (6). For $\omega_D \ll E_F$, Eq. (6) reads

$$\begin{aligned} \Delta_q(T) &= \oint_{\mathrm{FS}} V_{q,p}\Delta_p \int_0^{\omega_D} \frac{\tanh(E_p/2T)}{E_p} d\xi_p \frac{dS_p}{(2\pi\hbar)^D v_F} \\ &= \nu_F \left\langle V_{q,p}\Delta_p \int_0^{\omega_D} \frac{\tanh(E_p/2T)}{E_p} d\xi_p \right\rangle_p . \end{aligned} \tag{A32}$$

At $T = T_c$ [cf. Eqs. (A8)–(A10)] this formula gives

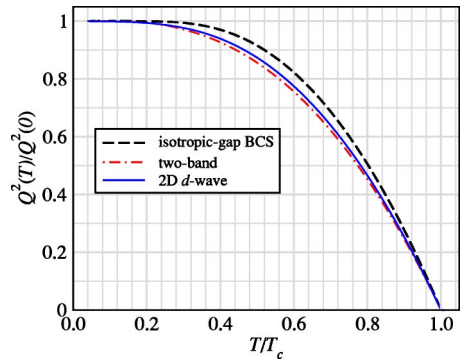

FIG. 9. (Color online) Squared reduced order parameter $Q^2(T)/Q^2(0)$ vs reduced temperature $t = T/T_c$ For the two-band model, the c_1 and δ parameters are chosen so as to simulating a d-wave CuO_2: $c_1 = 1/2$, $\delta = 2.41$.

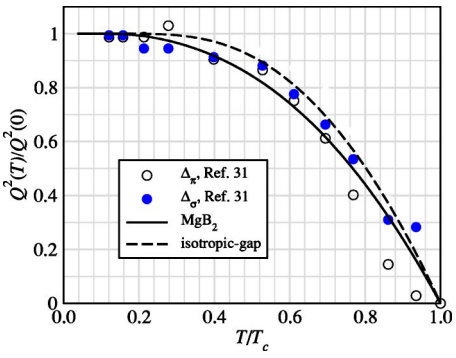

FIG. 10. (Color online) Squared reduced order parameter $Q^2(T)/Q^2(0)$ vs the reduced temperature $t=T/T_c$ for MgB_2 (solid line) with $c_1=0.44$, $\delta=7.1/2.8$. The experimental points for MgB_2 (circles) are digitized from Ref. 31.

$$\Delta_q(T_c) \approx \nu_F \ln\left(\frac{2\gamma\omega_D}{\pi T_c}\right)\langle V_{q,p}\Delta_p\rangle_p. \tag{A33}$$

Let us also mention the dimensions of the variables. Since the integration $\int\cdots[d^3p/(2\pi\hbar)^3]$ has a dimension of 1/volume, then $V_{q,p}$, being a Fourier component of potential energy, has dimension of energy$\times$volume. For example, the Coulomb potential e^2/r has a dimension of energy and its Fourier transformation

$$\frac{4\pi e^2}{k^2} = \int \frac{e^2}{r} e^{-i\mathbf{k}\cdot\mathbf{r}} d^3r \tag{A34}$$

has a dimension of energy$\times$volume. The same holds for the contact attraction in the BCS model potential $V(\mathbf{r})=-G\delta(\mathbf{r})$ having a constant Fourier component $-G$. The density of states ν_F has a dimension of (energy$\times$volume)$^{-1}$, Δ_p and E_p have a dimension of energy, and the Fermi surface averaging brackets $\langle\ldots\rangle$ represent a dimensionless operation.

Let the dimensionless parameter V_0 denotes the maximum eigenvalue of the problem

$$\langle V_{q,p}\chi_p\rangle_p = V_0\chi_q, \tag{A35}$$

and χ_p is the corresponding eigenvector, with normalization $\langle\chi_p^2\rangle=1$. The comparison of Eqs. (A35) and (A33) gives

$$T_c = \frac{2\gamma\omega_D}{\pi}\exp\left(-\frac{1}{\nu_F V_0}\right), \tag{A36}$$

which is identified with Eq. (A10) and we obtain

$$G = V_0 = \frac{\langle\chi_q V_{q,p}\chi_p\rangle_{q,p}}{\langle\chi_p^2\rangle_p}. \tag{A37}$$

As the maximal eigenvalue is sought, one can apply in this case the Krilov iterations

$$\chi_q^{(n+1)} \propto \langle V_{q,p}\chi_p^{(n)}\rangle_p, \quad \langle(\chi_p^{(n+1)})^2\rangle = 1, \tag{A38}$$

starting from some solutionlike trial vector $\chi_p^{(0)}$. Then the gap anisotropy function χ_p is just the limit of the Krilov iterations $\chi_p^{(\infty)}$.

For $T=0$, the gap equation (A32) gives

$$\Delta_q(0) = \left\langle V_{q,p}\ln\left(\frac{2\omega_D}{\tilde{Q}(0)|\tilde{\chi}_p|}\right)\Delta_p\right\rangle_p. \tag{A39}$$

Within the weak-coupling BCS approximation, in the integrant

$$\ln\left(\frac{2\omega_D}{|\Delta_p(0)|}\right) = \ln\left(\frac{2\omega_D}{\tilde{Q}(0)}\right) - \ln|\tilde{\chi}_p| \tag{A40}$$

the first term is much bigger than the second one. For details we refer to the original work by Pokrovsky,[1] but, roughly speaking, $\ln[2\omega_D/\Delta_p(0)]\approx\text{const}\gg 1$. Within the latter approximation for $\Delta_p(0)$ we obtain again the same eigenvalue problem and this constitutes the proof that the momentum dependence of the gap is rigid. Hence we derive the separation of the variables $\Delta_p(T)\approx Q(T)\chi_p$. When the term $\ln|\chi_p|$ in Eq. (A40) is small it can be treated perturbatively, and according to the normalization Eq. (A14) its influence diminishes. The properties of this approximative separation of the variables can be simulated by a factorizable kernel

$$V_{q,p} = \sum_n V_n\Psi_q^{(n)}\Psi_p^{(n)} \to V_0\chi_q\chi_p, \tag{A41}$$

where V_n are the eigenvalues and $\Psi_p^{(n)}$ are the corresponding eigenvectors of the problem

$$\langle V_{q,p}\Psi_p^{(n)}\rangle_p = V_n\Psi_q^{(n)}, \quad \langle|\Psi_p^{(n)}|^2\rangle = 1. \tag{A42}$$

In other words, the factorizable approximation [Eqs. (A41) and (7)] works well when the influence of smaller eigenvalues is small.

Generally speaking, the separability ansatz is a low-T_c approximation; T_c should be much smaller than all other energy parameters: energy cutoff, Debye frequency for phonon superconductors, exchange integrals for exchange mediated superconductivity, the Fermi energy, and the bandwidths. Room-temperature superconductivity is not yet discovered, but the good message is that we have still a simple approximation acceptably working for all superconductors. For theoretical models the accuracy of the separable approximation can be easily probed when investigating the angle between the order parameter at different temperatures, e.g.,

$$\arccos\frac{\langle\Delta_p^*(T)\Delta_p(T_c)\rangle}{\sqrt{\langle|\Delta_p(T)|^2\rangle\langle|\Delta_p(T_c)|^2\rangle}} \ll 1 \tag{A43}$$

or

$$\arccos\frac{\overline{\Delta_p^*(T)\Delta_p(T_c)}}{\sqrt{\overline{|\Delta_p(T)|^2}\,\overline{|\Delta_p(T_c)|^2}}} \ll 1. \tag{A44}$$

Those angles are just zero at T_c and the expressions for the specific heat jump and the GL coefficients is correct. Only for $T\to 0$ some small deviations can be observed, but in that case one can treat χ_p as a trial function in a variational approach.

The performed analysis shows that the separation of the variables Eq. (5) due to Pokrovsky[1] and consequent factorizable kernel Eq. (7) are tools to apply the weak-coupling

BCS approximation to anisotropic-gap superconductors. The factorizable kernel gives a simple solution to the gap equation, the nontrivial detail being that this separability can be derived by the BCS gap equation. The factorizable kernel has also been discussed by Markowitz and Kadanoff[5] and employed, e.g., by Clem,[43] to investigate the effect of gap anisotropy in pure and superconductors with nonmagnetic impurities. Factorizable kernels are now used in many works on exotic superconductors. However, in none of them is mentioned that the separability of the superconducting order parameter is an immanent property of the BCS theory.[1] The accuracy of the separable approximation is higher if the other eigenvalues of the pairing kernel are much smaller than the maximal one. This is likely to be the situation for the *s-d* model for layered cuprates,[4] where the *s-d* pairing amplitude J_{sd} is much bigger than the phonon attraction and the other interatomic exchange integrals. In order for us to clarify this important approach to the theory of superconductivity, we have given here a rather methodical derivation of the Pokrovsky theory.

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