Specific Heat and Thermal Conductivity in the Mixed State of MgB_2

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The specific heat C and the electronic and phononic thermal conductivities κ_e and κ_{ph} are calculated in the mixed state for magnetic fields H near H_{c2}, including the effects of supercurrent flow and Andreev scattering. The resulting function $C(H)$ is nearly linear while $\kappa_e(H)$ exhibits an upward curvature near H_{c2}. The slopes decrease with impurity scattering which improves the agreement with the data on MgB_2. The ratio of phonon relaxation times $\tau_n/\tau_s = g(\omega_0, H)$ for phonon energy ω_0 is smeared out around $\omega_0 = 2\Delta$ and tends to one for increasing H. This leads to a rapid reduction of $\kappa_{ph}(H)$ in MgB_2 for relatively small fields due to the rapid suppression of the smaller energy gap.

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Numerous experiments indicate that the superconducting state of MgB_2 ($T_c = 40$ K) [1] is a conventional s-wave pairing state mediated by phonon exchange. Nevertheless, the theoretical explanation of physical quantities is demanding because two energy gaps are formed where the larger gap Δ_1 is associated with the nearly cylindrical σ sheets of the Fermi surface and the smaller gap Δ_2 with the three-dimensional π sheets. Analysis of the temperature dependence of the measured thermal conductivity in the basal plane of MgB_2 [2] gives evidence for two gaps on different Fermi surface sheets. The situation is complicated because the thermal conductivity κ is a sum of an electronic part κ_e and the phononic or lattice conductivity κ_{ph}. In Ref. [2] κ_e and κ_{ph} were calculated with help of the BCS theory [3], where κ_e is limited by elastic scattering (scattering by phonons is omitted) and κ_{ph} is limited by electron scattering. This theory for κ_{ph} is supplemented by adding to the phonon relaxation rate due to scattering by electrons, the relaxation rates due to scattering by point defects [4], and other defects. Note that the peak in κ_{ph} below T_c in the cuprate superconductors has been fitted by including scattering by sample boundaries, sheetlike faults, and dislocations [5].

Recently, the ab-plane thermal conductivity of MgB_2 has been measured as a function of magnetic field H with orientations both parallel and perpendicular to the c axis [6]. At low temperatures, $\kappa(H)$ drops steeply for increasing H up to a relatively low field which we denote by $H_{c2}^{(2)}$ (~ 1 kOe), and then it rises continuously up to H_{c2} ($\simeq$ 30 kOe for $\mathbf{H} \parallel \mathbf{c}$). The first drop of κ is interpreted as due to the behavior of $\kappa_{ph}(H)$ which is caused by a strong suppression of the smaller gap Δ_2 by relatively small fields. This leads to a rapid increase in the number of those quasiparticles that dominate the scattering of phonons [2]. The rapid suppression of the smaller gap can be explained in terms of a two-band model with different energy gaps where the smaller gap is induced by Cooper pair tunneling from the band with the larger gap [7]. The observed increase of $\kappa(H)$ above $H_{c2}^{(2)}$ is attributed to the increase of $\kappa_e(H)$ because κ_{ph} has already reached its normal-state value [6]. Since this field dependence of $\kappa_e(H)$ at low temperatures is qualitatively similar to that of the specific heat coefficient $\gamma(H)$ [8,9], it is concluded that the growth of $\kappa_e(H)$ is due to the rapid increase of quasiparticles in the vortex cores associated with the larger energy gap.

In this Letter, we present theories for the specific heat and the electronic and phononic thermal conductivities in the vortex state for applied fields near the upper critical field H_{c2}. For simplicity, we consider only one isotropic s-wave pairing gap either on a cylindrical Fermi surface with $\mathbf{H} \parallel \mathbf{c}$, or on a spherical Fermi surface. Our goal is to explain the measured quantities $\gamma(H)$ and $\kappa_e(H)$ near H_{c2} ($\simeq$ 30 kOe), and $\kappa_{ph}(H)$ below the effective upper critical field $H_{c2}^{(2)}$ (~ 1 kOe) for the vortex lattice associated with the smaller energy gap. Our theories are based on the normal and anomalous Green's functions G and F obtained from the Gorkov integral equations with kernels given by the product of Abrikosov vortex lattice order parameters $\Delta(\mathbf{r_1})\Delta^*(\mathbf{r_2})$ and the phase factor due to the magnetic field [10]. These Green's functions depend sensitively on $\sin\theta$, where θ is the angle between the quasiparticle momentum $\mathbf{p}$ and the magnetic field $\mathbf{H}$. For $\theta \rightarrow 0$, G and F tend to the Green's functions for a BCS superconductor while, for $\theta \rightarrow \pi/2$, they take into account the effects of supercurrent flow and Andreev scattering due to the vortex lattice. This theory has been applied previously to calculate $\kappa_e(T, H)$ for energy gaps with line nodes similar to those occurring in the high-T_c cuprates and Sr_2RuO_4 [11].

A simplified version of the theory in Ref. [10], which has been derived from the Eilenberger equations [12], yields for the spatial average of the density of states:

$$N(\omega, \theta)/N_0 \equiv A(\Omega; \tilde{\Delta}, \theta) = \mathrm{Re}\left[1 + \frac{8\tilde{\Delta}^2}{\sin^2\theta}[1 + i\sqrt{\pi}\, z\, w(z)]\right]^{-1/2}. \quad (1)$$

The quantities appearing here are defined as follows: $z = 2[\Omega\tilde{\Delta} + i(\Lambda/v)\Gamma]/\sin\theta$ with $\theta = \angle(\mathbf{p}, \mathbf{H})$, $\Lambda = (2eH)^{-1/2}$, $\tilde{\Delta} = \Delta\Lambda/v$, $\Omega = \omega/\Delta$, $\tilde{\Delta}^2 = (H_{c2} - H)/6\beta_A H$, $\Delta^2 = \Delta_0^2(T)[1 - (H/H_{c2})]$, and $w(z) = \exp(-z^2)\mathrm{erfc}(-iz)$. Here v is the Fermi velocity, β_A is the Abrikosov parameter which we take as 1.2, $\Delta_0(T)$ is the BCS gap, and Γ is the normal-state impurity scattering rate. The specific heat C is given by $C = N_0 T \int_0^\infty dx x^2 \,\mathrm{sech}^2(x/2) A(Tx/\Delta)$. At low temperatures ($T \ll \Delta$), $C = \gamma_s(H)T$, where the coefficient $\gamma_s(H)$ is proportional to $A(\Omega = 0)$. In Fig. 1, we have plotted $A(\Omega = 0)$ versus H/H_{c2} for $\sin\theta = 1$ corresponding to a cylindrical Fermi surface and $\mathbf{H} \parallel \mathbf{c}$, and several impurity scattering rates $\delta \equiv \Gamma/\Delta_0$. A is seen to be nearly linear near H_{c2} with a slope at H_{c2} that decreases for increasing δ. In Fig. 1, we also show the angular average $\bar{A} = \int_0^{\pi/2} d\theta \sin\theta A(\theta)$ which corresponds to a three-dimensional Fermi surface. Comparison with the solid curves in Fig. 1 shows that the slopes at H_{c2} are decreased by the angular average. Note that our results are strictly valid only in the vicinity of H_{c2}. However, solution of the Eilenberger equations for a vortex lattice shows that the spatial average of the resulting density of states is well approximated by $A(\Omega)$ for fields down to about $(1/2)H_{c2}$ [13]. The solid curve of A vs H/H_{c2} for $\delta = 0.5$ in Fig. 1 agrees qualitatively with the measured field dependence of the specific heat coefficient $\gamma_s(H)$ at low temperatures and fields near H_{c2} [8,9].

We turn now to the theory of the electronic thermal conductivity κ_e in the vortex state near H_{c2} which has been developed in Ref. [11]. These expressions are easily modified to apply to an isotropic s-wave pairing state and a field along the c axis. Employing the expression valid at low temperatures, we obtain for the ratio κ_{es}/κ_{en} as a function of H/H_{c2} the plots shown in Fig. 2 for constant $\sin\theta = 1$ and impurity scattering rates $\delta = 0.1$, 0.2, and 0.5. These plots exhibit upward curvatures with decreasing slopes at H_{c2} for increasing values of δ. In Fig. 2, we have also plotted the corresponding results for the angular averages over θ of κ_{es}/κ_{en}. Comparison with the measured $\kappa(H)$ near H_{c2}, which is presumably dominated by the field dependence of $\kappa_e(H)$ [6], shows that the measured upward curvature towards H_{c2} is qualitatively best described by the upper solid curve in Fig. 2 for the relatively large impurity scattering rate $\delta = 0.5$.

It was argued in Ref. [6] that the similar field dependencies of the specific heat and electronic thermal conductivity can be explained in terms of the relationship $\kappa_e = C_e v_F \ell/3$, where ℓ is the mean-free path. In fact, our theoretical expression for κ_e has a similar form if one sets $\ell = v_F \tau_e$, where $\tau_e = 1/\mathrm{Im}\xi_0$ with $\mathrm{Im}\xi_0 = \gamma + \gamma_A$ [11]. Here γ is the impurity scattering rate and γ_A is the scattering rate due to Andreev scattering of the quasiparticles by the vortices. γ_A is shown as a function of angle θ for different values of Ω and $\tilde{\Delta}$ in Ref. [14]. These plots show that, for extended states ($\Omega \geq 1$), γ_A increases from zero as θ increases from 0 to $\pi/2$. This means that the Andreev scattering rate has a maximum for quasiparticles moving perpendicular to the vortex axis. For increasing field (decreasing $\tilde{\Delta}$), γ_A decreases which has the effect that the curve for κ_{es}/κ_{en} exhibits an upward curvature in comparison to C_e which has a slight downward curvature for increasing field.

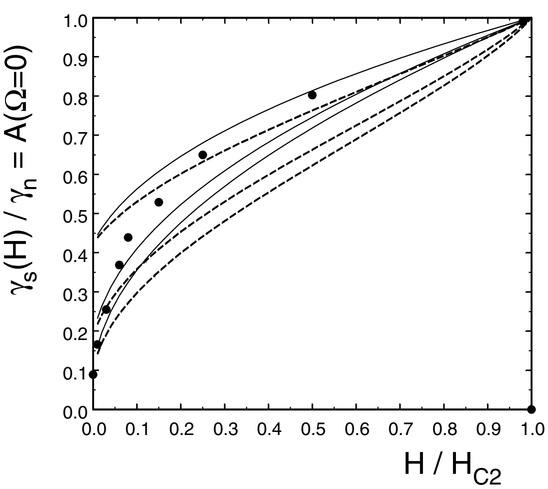

FIG. 1. Reduced density of states at zero energy, $A(\Omega = 0, H) = \gamma_s(H)/\gamma_n$ vs H/H_{c2} for impurity scattering rates $\delta = \Gamma/\Delta_0 = 0.1$, 0.2, and 0.5 (from bottom to top). Solid curves for angle $\theta = \pi/2$ corresponding to $\mathbf{H} \parallel \mathbf{c}$ for a cylindrical Fermi surface (θ is the angle between the quasiparticle momentum $\mathbf{p}$ and the field $\mathbf{H}$). Dashed curves for the average of A over θ corresponding to a spherical Fermi surface. The dots are reduced data from Ref. [8] for MgB_2 at $T = 3$ K.

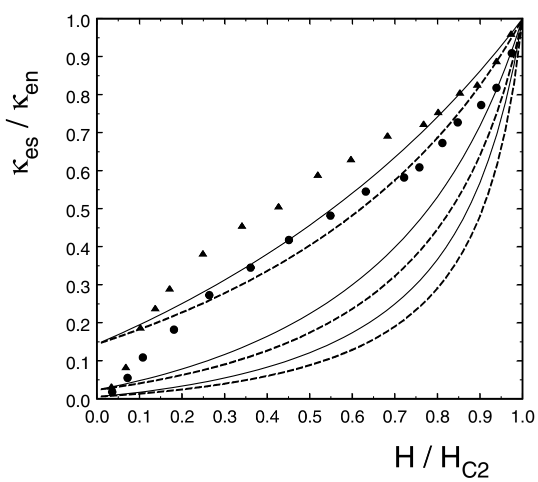

FIG. 2. Electronic thermal conductivity ratio κ_{es}/κ_{en} at low temperatures vs H/H_{c2} for impurity scattering rates $\delta = 0.1$, 0.2, and 0.5 (from bottom to top). Notation as in Fig. 1: Solid curves for angle $\theta = \pi/2$. Dashed curves for the average over θ. The dots (triangles) are reduced data from Ref. [6] for MgB_2 at $T = 7.94$ K ($T = 5.13$ K).

Until now, there exists only a phenomenological theory for the phonon heat transfer in the mixed state where the phonons are scattered by vortices consisting of normal-state cylinders [15]. We develop here the microscopic theory of κ_{ph} (limited by electron scattering) in the vortex state in close analogy to the theory for the BCS state [3]. In that case, the sum of probabilities for absorption and emission of phonons by quasiparticles yields a relaxation rate $1/\tau_s$ for a phonon of energy ω_0 which is proportional to the integral over quasiparticle energy E of the expression $|EE'/\varepsilon\varepsilon'|[1 - \Delta^2/EE'][f(E/T) - f(E'/T)]$. Here, $E/\varepsilon = E/(E^2 - \Delta^2)^{1/2}$ is the density of states, $E' = E + \omega_0$, and $f(E/T)$ is the Fermi function. In the mixed state near H_{c2}, the density of states E/ε is replaced by $A(\Omega)$ as given in Eq. (1). The coherence term $(\Delta/\varepsilon)(\Delta/\varepsilon')$, which arises from the matrix elements for quasiparticle scattering, is replaced by $FF^\dagger$, where the anomalous Green's function F is given in Ref. [11]. The spectral function of F yields the following analog of Δ/ε:

$$B(\Omega; \tilde{\Delta}, \theta) = \mathrm{Re}\left[\frac{-i\sqrt{\pi}\,2(\tilde{\Delta}/\sin\theta)w(z)}{\{1 + (8\tilde{\Delta}^2/\sin^2\theta)[1 + i\sqrt{\pi}\,z\,w(z)]\}^{1/2}}\right]. \tag{2}$$

The argument z was defined below Eq. (1). The functions $A(\Omega)$ and $B(\Omega)$ are even and odd in Ω. For $\theta \to 0$, they tend to the BCS functions $\omega/(\omega^2 - \Delta^2)^{1/2}$ and $\Delta/(\omega^2 - \Delta^2)^{1/2}$, respectively. In this way, we obtain the following for the ratio of phonon relaxation times in the normal and superconducting states (denoted by g in Refs. [2,3,5]):

$$\begin{aligned}\tau_n/\tau_s &= g(\Omega_0)\\ &= [1 - \exp(-\Omega_0\Delta/T)](2/\Omega_0)\int_0^\infty d\Omega f[(\Omega - \Omega_0/2)\Delta/T]f[-(\Omega + \Omega_0/2)\Delta/T]\\ &\quad\times[A(\Omega - \Omega_0/2)A(\Omega + \Omega_0/2) - B(\Omega - \Omega_0/2)B(\Omega + \Omega_0/2)].\end{aligned} \tag{3}$$

The quantity $\Omega_0 = \omega_0/\Delta$ is the phonon energy ω_0 divided by the effective gap $\Delta = \Delta(H)$. For $T \ll \Delta$, the function ff in the integrand of Eq. (3) is approximately one in the range from $\Omega = 0$ to $\Omega_0/2$ and zero above $\Omega_0/2$. In Fig. 3, we show some examples of the function $g(\Omega_0)$ for various parameter values. For increasing $\tilde{\Delta}$, or decreasing field, the function g tends to the BCS step function which is zero in the range from $\Omega_0 = 0$ to 2, and $\pi/2$ for $\Omega_0 > 2$ (see Fig. 1 of Ref. [5]). The physical meaning of g at low temperatures for the BCS superconductor is that the minimum energy of a phonon for creating a pair of quasiparticles is $\omega_0 = 2\Delta$. Figure 3 shows that, for increasing field, the relaxation rate is more and more smeared out and the ratio τ_n/τ_s tends to one. A similar effect occurs for increasing impurity scattering rate δ (see the dashed curve in Fig. 3).

The expression for the phonon thermal conductivity limited by electron scattering and several other scattering processes is given by [5]

$$\kappa_{ph} = At^3\int_0^\infty dx\frac{x^4\,e^x}{(e^x - 1)^2}[1 + \alpha t^4x^4 + \beta t^2x^2 + \delta tx + \gamma txg(xT/\Delta)]^{-1}. \tag{4}$$

Here $x = \omega_0/T$, $t = T/T_c$, and the coefficients A, α, β, δ, and γ refer to scattering by sample boundaries, point defects, sheetlike faults, dislocations, and quasiparticles, respectively. For $t \ll 1$ and $T \ll \Delta$, the argument of $g(\Omega_0)$ in Eq. (4) is approximately equal to zero. Taking the limit $\Omega_0 \to 0$ in Eq. (3) and noting that the coherence term B vanishes at $\Omega_0 = 0$, we obtain $g(\Omega_0 = 0) = [A(\Omega_0 = 0, \tilde{\Delta}, \theta)]^2$. For constant $\theta = \pi/2$, this expression yields the field dependence of τ_n/τ_s for the case $\mathbf{H} \parallel \mathbf{c}$ and a cylindrical Fermi surface. For a three-dimensional Fermi surface, which is presumably more appropriate for the quasiparticles associated with the smaller gap in MgB_2, we have to multiply $[A(0, \theta)]^2$ by $\sin\theta$ and integrate over θ from 0 to $\pi/2$. In Fig. 4, we have plotted our results for g at $\theta = \pi/2$ and for the angular average of g vs H/H_{c2} for impurity scattering rates $\delta = 0.1$ and 0.5.

The measured κ_{ph} at $H = 0$ [2] has been analyzed in terms of an expression which is equivalent to our Eq. (4), apart from the term proportional to β. By inserting two different contributions for the electron scattering term γ

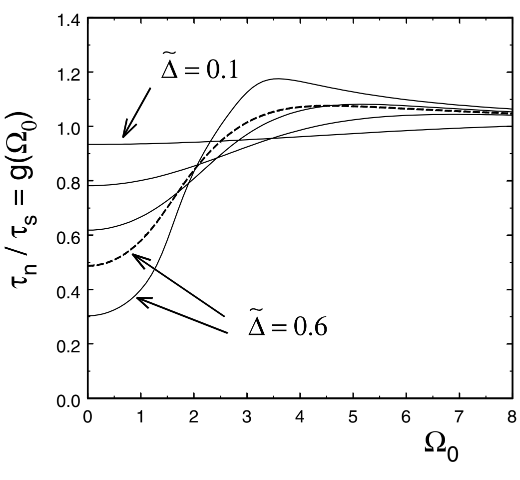

FIG. 3. Ratio of phonon relaxation times $\tau_n/\tau_s = g(\Omega_0)$ due to electron scattering at low temperatures vs $\Omega_0 = \omega_0/\Delta$, where ω_0 is the phonon energy and $\Delta = \Delta(H)$ the effective energy gap. From top to bottom, $\tilde{\Delta} = 0.1$, 0.2, 0.3, and 0.6, corresponding to $H/H_{c2} = 0.93$, 0.78, 0.61, and 0.28. Also, $\delta = 0.1$ and $\theta = \pi/2$ (notation of Fig. 1). The dashed curve refers to $\tilde{\Delta} = 0.6$ and impurity scattering rate $\delta = 0.5$.

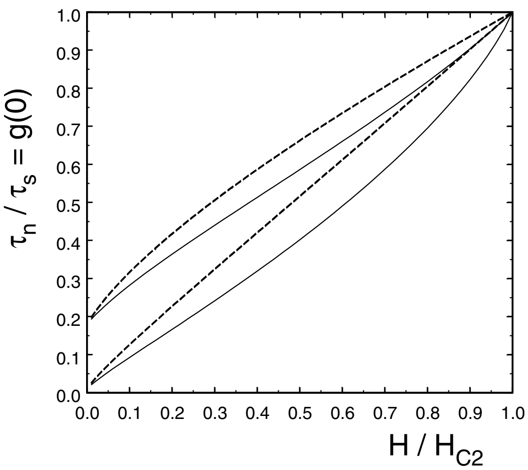

FIG. 4. Ratio $\tau_n/\tau_s = g(\Omega_0 = 0, H)$ vs H/H_{c2} for $\delta = 0.1$ (lower curves) and $\delta = 0.5$ (upper curves) with the notation of Fig. 3. This quantity determines the reduction of the phonon thermal conductivity at low temperatures due to the increase of scattering by quasiparticles. The solid curves are the average of g over θ corresponding to a spherical Fermi surface and the dashed curves are g for constant $\theta = \pi/2$.

corresponding to different gaps Δ_1 and Δ_2, the fitting procedure indicated that the dominant part of the scattering of phonons by electrons is provided by that part of the electronic excitation spectrum experiencing the smaller gap, Δ_2. According to the two-band theory of Ref. [7], this smaller gap is suppressed by a relatively small effective upper critical field $H_{c2}^{(2)}$ which leads to the measured fast drop of $\kappa_{ph}(H)$ as H increases from 0 to $H_{c2}^{(2)}$ [6]. We conclude that the measured field dependence of $\kappa_{ph}(H)$ below $H_{c2}^{(2)}$ at low temperatures can be explained by inserting in Eq. (4) the values of the various constants obtained for $H = 0$ and, for $\tau_n/\tau_s = g(H)$, the angular average of $g(\Omega_0 = 0) = [A(\Omega_0 = 0, \tilde{\Delta}, \theta)]^2$. The behavior of $g(H)$, which determines the form of the fast reduction of $\kappa_{ph}(H)$, depends on the impurity scattering rate δ (see Fig. 4).

An important effect on the upward curvature of κ_{es}/κ_{en} arises from the decrease of the Andreev scattering rate γ_A with increasing field. This decrease is given approximately by the expression $\gamma_A / \Delta_0 = \sqrt{\pi}(\tilde{\Delta}^2/\sin\theta) \times \exp[-(2\Omega\tilde{\Delta}/\sin\theta)^2]$, where $\tilde{\Delta}^2 \sim (H_{c2} - H)/H$. It is interesting that the exponent in this expression, in particular, the term $(\sin\theta)^{-2}$, is similar to the exponent in the scattering rate $1/\tau_v$ which has been derived previously [16]. In that model, a quasiparticle is converted into a hole due to Andreev reflection by vortex screening currents. This process corresponds just to the imaginary part of the self-energy calculated in Ref. [10].

Our theory is strictly valid only for fields near the upper critical field H_{c2}. However, recent numerical solutions of the quasiclassical Eilenberger equations for the Abrikosov vortex lattice [13] have shown that the analytical expressions for the density of states [10,12] [here the function $A(\Omega)$] yield at low energies impressively good results over the whole range of fields down to H_{c1}. These results for low energies are important for the calculation of thermodynamic quantities. We expect that this is also true for the function $B(\Omega)$, the spectral function of the anomalous Green's function.

In conclusion, we have employed microscopic theories for the electronic specific heat $C(H)$ and the thermal conductivity $\kappa_e(H)$ and developed a microscopic theory for the phononic thermal conductivity $\kappa_{ph}(H)$ to explain the measured field dependence of these quantities in the mixed state of MgB_2. We find that impurity and Andreev scattering, as well as Fermi surface anisotropy, give rise to large effects. For sufficiently large impurity scattering rate, one can approximately fit the data for $C(H)$ and $\kappa_e(H)$ for MgB_2 over a broad field range below H_{c2}. Our new theory for $\kappa_{ph}(H)$ is capable of describing the observed rapid reduction of the total κ of MgB_2 for small fields if this is actually caused by suppression of a second smaller energy gap.

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[1] J. Nagamatsu, N. Nakagawa, T. Muranaka, Y. Zenitani, and J. Akimitsu, Nature (London) **410**, 63 (2001).
[2] A.V. Sologubenko, J. Jun, S. M. Kazakov, J. Karpinski, and H. R. Ott, cond-mat/0111273.
[3] J. Bardeen, G. Rickayzen, and L. Tewordt, Phys. Rev. **113**, 982 (1959).
[4] P. G. Klemens and L. Tewordt, Rev. Mod. Phys. **36**, 118 (1964).
[5] L. Tewordt and Th. Wölkhausen, Solid State Commun. **70**, 839 (1989).
[6] A.V. Sologubenko, J. Jun, S. M. Kazakov, J. Karpinski, and H. R. Ott, cond-mat/0201517.
[7] N. Nakai, M. Ichioka, and K. Machida, J. Phys. Soc. Jpn. **71**, 23 (2002).
[8] A. Junod, Y. Wang, F. Bouquet, and P. Toulemonde, cond-mat/0106394.
[9] H. D. Yang *et al.*, Phys. Rev. Lett. **87**, 167003 (2001).
[10] U. Brandt, W. Pesch, and L. Tewordt, Z. Phys. **201**, 209 (1967).
[11] L. Tewordt and D. Fay, Phys. Rev. B **64**, 24528 (2001).
[12] W. Pesch, Z. Phys. B **21**, 263 (1975).
[13] T. Dahm, S. Graser, C. Iniotakis, and N. Schopohl, cond-mat/0205163.
[14] L. Tewordt and D. Fay, Phys. Rev. B **65**, 104510 (2002).
[15] J. B. Sousa, Physica (Utrecht) **55**, 507 (1971).
[16] F. Yu, M. B. Salamon, A. J. Leggett, W. C. Lee, and D. M. Ginsberg, Phys. Rev. Lett. **74**, 5136 (1995).