Superconductive specific-heat transition in a magnetic field

Alan J. Bray

The Physics Laboratories, The University of Kent, Canterbury, Kent, England
*and Center for Theoretical Physics University of Maryland, College Park, Maryland 20742**

(Received 28 January 1974)

The specific-heat transition of bulk and thin-film superconductors in a uniform magnetic field is studied within the Ginzburg-Landau model using a screening treatment of the order-parameter fluctuations. For the bulk case, reasonable quantitative agreement is obtained with the experimental results of Barnes and Hake.

I. INTRODUCTION

In this paper we investigate the effect of a uniform magnetic field on the specific-heat transition of bulk and thin-film superconductors. We work within the Ginzburg-Landau (GL) theory which starts from the expression for the free energy $F_{\rm GL}$ in terms of the local order parameter $\psi(\vec{r})$,

$$f\{\psi\} = \frac{F_{\rm GL}\{\psi\}}{T} = \int d^3r\{\alpha|\psi|^2 + \delta|[-i\vec{\nabla} - 2e\vec{A}(\vec{r})]\psi|^2 + \tfrac{1}{2}\beta|\psi|^4\}, \quad (1.1)$$

where $\vec{A}(\vec{r})$ is the vector potential and α, δ, β are the usual GL parameters incorporating an extra factor $1/T$. Hence[1]

$$\alpha = \frac{\delta\epsilon}{\xi^2(0)}, \quad \delta = \frac{1}{2mT}, \quad \beta = \frac{\xi_0^2}{nm\xi^4(0)T}, \quad \epsilon = \frac{T-T_c}{T_c}, \quad (1.2)$$

where

$$\xi(0) = \xi_0 \simeq 0.133 k_F/mT_c \text{ in the pure limit } (l \gg \xi_0)$$
$$\simeq 0.99(l\xi_0)^{1/2} \text{ in the dirty limit } (l \ll \xi_0) \quad (1.3)$$

is the (temperature-independent) coherence length. (Note that our definition of ξ_0 differs from that common in the literature.) Here k_F is the Fermi momentum, l is the electron mean free path, and n is the electron density; e and m are the charge and mass of the electron respectively and we use units such that $\hbar = k_B = c = 1$ throughout.

The thermodynamic properties of the system are obtained from the partition function which is given by a functional integral (over all order-parameter configurations) of a Boltzmann factor with Eq. (1.1) in the exponent:

$$Z_{\rm GL} = \int d^2\psi(\vec{r})e^{-f\{\psi\}} . \quad (1.4)$$

To calculate the specific heat we will make, as a first step, the usual assumption that all the temperature dependence enters through the parameter α, and set any T which appears explicitly equal to T_c. This is usually a good approximation for superconductors since transition widths are typically so narrow. It also has the advantage of leading to a "one-parameter" model. Hence we write for the entropy $S = \partial \ln Z_{\rm GL}/\partial\alpha$ and for the specific heat $C = \partial S/\partial\alpha$. We normalize the result by dividing by the discontinuity in the specific heat at zero field predicted by mean-field theory. Mean-field theory gives

$$|\psi|^2 = 0 \qquad \alpha > 0$$
$$= -\alpha/\beta, \quad \alpha < 0$$

giving

$$f = 0 \qquad \alpha > 0$$
$$= -v\alpha^2/2\beta, \quad \alpha < 0 \quad (1.5)$$

and

$$C = -\frac{\partial^2 f}{\partial\alpha^2} = 0 \qquad \alpha > 0$$
$$= v/\beta, \quad \alpha < 0 .$$

The mean-field discontinuity at the transition is $\Delta C = v/\beta$ where $v = L_xL_yL_z$ is the volume of the system. To calculate the fluctuation specific heat we use the following relation for the entropy which follows from Eqs. (1.1) and (1.4):

$$S = \frac{\partial \ln Z_{\rm GL}}{\partial\alpha} = -\int d^3r\langle|\psi(\vec{r})|^2\rangle . \quad (1.6)$$

The angular brackets have the usual meaning that for any function $A(\psi)$,

$$\langle A(\psi)\rangle = \int d^2\psi A(\psi)e^{-f\{\psi\}} \Big/ \int d^2\psi e^{-f\{\psi\}} .$$

The normalized specific heat becomes

$$\frac{C}{\Delta C} = \frac{\beta}{v}\frac{\partial S}{\partial\alpha} = -\frac{\beta}{v}\frac{\partial}{\partial\alpha}\int d^3r\langle|\psi(\vec{r})|^2\rangle . \quad (1.7)$$

II. FREE FLUCTUATION THEORY

The effect of a uniform magnetic field on the specific heat transition was first investigated theoretically by Lee and Shenoy.[2] They used "free-fluctuation theory," that is they neglected the fourth-order term in Eq. (1.1), to calculate the fluctuation specific heat above T_c. Their basic physical idea is the following. In a uniform magnetic field the fluctuating electron pairs move in Landau orbitals characterized by K_z and n. The transition temperature $T_{c2}(H)$ is the temperature at which the $n=0$ Landau orbital becomes stable, giving rise to the vortex state. Just above $T_{c2}(H)$ the lowest, $n=0$, orbital dominates the fluctuation contributions and as a result only one degree of freedom remains, namely, that along the z direction. A bulk superconductor thus behaves like an array of one-dimensional rods parallel to the field with the number of rods per unit area given by eH/π, the Landau degeneracy factor for particles of charge $2e$. The fluctuation specific heat is then proportional to the field and becomes one dimensional in nature, diverging within free-fluctuation theory as $\alpha^{-3/2}$. For a thin film, with the field perpendicular to the plane of the film, the K_z degree of freedom is suppressed and the system becomes effectively zero dimensional. The specific heat diverges within free-fluctuation theory as α^{-2}.

These results may be derived quantitatively from Eq. (1.1) by expanding the order parameter in terms of the Landau orbitals $\langle\vec{r}\,|\,n, K_z, q\rangle$ instead of the usual plane waves. We write

$$\psi(\vec{r}) = \sum_{n, K_z, q} \phi_{n, K_z, q} \langle\vec{r}\,|\,n, K_z, q\rangle , \qquad (2.1)$$

where the $\langle\vec{r}\,|\,n, K_z, q\rangle$ are the normalized eigenfunctions[3] of a free particle of charge $2e$ in a magnetic field H (assumed in the z direction). Substituting Eq. (2.1) into (1.1), neglecting the term in $|\psi|^4$, yields

$$f\{\phi\} = \sum_{n, K_z, q} \{\alpha + \delta K_z^2 + (2n+1)2e\delta H\}\,|\phi_{n, K_z, q}|^2 , \qquad (2.2)$$

and therefore

$$\langle|\phi_{n, K_z, q}|^2\rangle = \{\alpha + \delta K_z^2 + (2n+1)2e\delta H\}^{-1} .$$

From Eqs. (1.7) and (2.1) the specific heat is given by

$$\frac{C}{\Delta C} = -\frac{\beta}{v}\frac{\partial}{\partial\alpha}\sum_{n, K_z, q}\langle|\phi_{n, K_z, q}|^2\rangle = \frac{\beta}{v}\sum_{n, K_z, q}\frac{1}{(\alpha_H + \delta K_z^2 + 2nh)^2} , \qquad (2.3)$$

where $h = 2e\delta H$ and $\alpha_H = \alpha + h$. The transition temperature $T_{c2}(H)$ is given within the GL theory by the condition $\alpha_H = 0$. In agreement with the general arguments above we see that close to the transition, when $\alpha_H \ll h$, the sum over n in Eq. (2.3) is dominated by the single term $n=0$. The sum over K_z is performed by making the replacement $\sum_{K_z} \to L_z\int_{-\infty}^{\infty}(dK_z/2\pi)$ and that over q is performed by merely multiplying by the Landau degeneracy factor $(eH/\pi)L_xL_y$. Hence for a bulk system we obtain

$$\text{(three dimensions)}\quad \frac{C}{\Delta C} = \frac{eH}{\pi}\,\frac{\beta}{4\alpha_H(\alpha_H\delta)^{1/2}} . \qquad (2.4)$$

For a thin film the K_z degree of freedom is suppressed. The sum over K_z is dominated by the single term $K_z = 0$ to give

$$\text{(two dimensions)}\quad \frac{C}{\Delta C} = \frac{eH}{\pi}\,\frac{\beta}{d\alpha_H^2} , \quad d = L_z = \text{film thickness}. \qquad (2.5)$$

Defining the transition width as that value of $\epsilon_H[=\alpha_H\xi^2(0)/\delta]$ for which $C = \Delta C$ we see that the width varies as $H^{2/3}$ and $H^{1/2}$ for the three- and two-dimensional cases, respectively. By broadening the transition the application of a magnetic field renders the critical region more accessible to experiment. Note that in the low-field limit, $h \ll \alpha_H$, the sum over n in Eq. (2.3) can be converted to an integral[2] to recover the usual zero-field results.[4]

Recently, some doubt has been cast on the validity of Eq. (1.1), notably in connection with the calculation of the fluctuation enhanced diamagnetism.[5,6] The microscopic derivation[7] of Eq. (1.1) assumes that $\psi(\vec{r})$ is a slowly varying function of position in the sense that $|\vec{\nabla}\psi/\psi| \ll \xi(0)^{-1}$. In using the usual GL free-energy functional we are assuming that low-energy fluctuations provide the dominant contribution to physical quantities near the transition. In the case of the magnetization this assumption does not hold. High-energy fluctuations are important and consequently a more complete form of the free-energy functional is required, which turns out to be nonlocal in character. We refer the reader to the papers of Lee and Payne[5] and Kurkijarvi *et al.*[6] for further details. For the specific-heat calculations of this paper we will assume that Eq. (1.1) adequately describes the free-energy functional in a magnetic field. The experiments of Barnes and Hake,[8,9] which we discuss later, were carried out on very dirty samples for which the local theory should in any case be valid.[5,6]

The obvious next step following the free fluctuation theory of Lee and Shenoy is the use of the Hartree approximation[10] to allow for interactions between order parameter fluctuations. Such a program has been carried out by Grossman *et al.*[11] and by Hassing, Hake, and Barnes.[9] The latter authors have compared their predictions with the experimental results of Barnes and Hake[8] on dirty bulk superconductors. The results are disappointing. The theoretical curves show no indication of the peaking behavior exhibited by the experimental points. Furthermore, the measured jump in the specific heat at the transition falls off more quickly with increasing magnetic field than is predicted by theory. To overcome the first of these shortcomings we shall apply in Sec. III a variant of the "screening approximation" of Bray and Rickayzen.[12,13] In this treatment of the GL model, interactions between fluctuations of the order parameter are screened by processes in which virtual fluctuations are created and destroyed. Since this approximation gives excellent results when used to derive the specific heat of "real" zero[1]- and one-dimensional[12] systems (for which exact results are known), it may be hoped that it does so for the "pseudo" zero- and one- dimensional systems considered here. In fact we find that a screening treatment of the order parameter fluctuations does indeed produce the peaking behavior observed by Barnes and Hake. The sharp falloff of the specific-heat jump with increasing field, however, still requires explanation.

III. SCREENING THEORY

In this section we present a theory of the specific-heat transition of bulk and thin film superconductors in a magnetic field based on a screening treatment of the order-parameter fluctuations. Preliminary results have been reported elsewhere.[14] We summarize below the assumptions made: (i) All the temperature dependence of the problem is contained in the reduced relative temperature $\epsilon=(T-T_c)/T_c$. (ii) Vortex-lattice structure can be ignored in the critical region. (iii) Only the lowest, $n=0$, Landau orbital is important in the critical region. (iv) The interacting fluctuation system is well described, even in strong magnetic fields, by the free-energy-functional equation (1.1). Assumption (i) is made for simplicity: it ensures that we have essentially a one-parameter model. In making detailed comparisons with experiment in Sec. IV this assumption will be relaxed.

Our starting point is the free-energy-functional equation (1.1). As in the free fluctuation theory of Lee and Shenoy we expand $\psi(\vec{r})$ in terms of the Landau orbitals $\langle\vec{r}\,|\,n, K_z, q\rangle$ according to Eq. (2.1). Here, however, we retain the fourth-order term in the free-energy functional. In accordance with assumption (iii) above we retain $n=0$ terms only to give

$$f=\sum_{K_z,q}(\alpha_H+\delta K_z^2)|\phi_{K_z,q}|^2+\tfrac{1}{2}\beta\sum_{\substack{K_{1z},K_{2z},K_{3z},K_{4z}\\ q_1,q_2,q_3,q_4}}\phi^*_{K_{1z},q_1}\phi^*_{K_{2z},q_2}\times\phi_{K_{3z},q_3}\phi_{K_{4z},q_4}\int d^3r\langle\vec{r}\,|\,K_{1z},q_1\rangle^*\times\langle\vec{r}\,|\,K_{2z},q_2\rangle^*\langle\vec{r}\,|\,K_{3z},q_3\rangle\langle r\,|\,K_{4z},q_4\rangle\,.$$

The Landau eigenfunctions are given by[3]

$$\langle\vec{r}\,|\,K_z,q\rangle=Ae^{i(qy+K_zz)}u(q,x)\,,$$

where $u(q,x)$ is the ground-state harmonic-oscillator wave function centered on $x_0=\delta q/h$ (recall $h=2e\delta H$), and A is the normalization constant. Explicitly,

$$\langle\vec{r}\,|\,K_z,q\rangle=Ae^{i(qy+K_zz)}e^{-(h/2\delta)(x-x_0)^2}\,.$$

Normalization over a cuboid of sides L_x, L_y, L_z gives

$$A^2=(1/L_yL_z)(h/\pi\delta)^{1/2}\,.$$

Hence the coefficient of the fourth-order term in f is given by

$$\tfrac{1}{2}\beta A^4\int\int dz\,dy\,e^{i(q_3+q_4-q_1-q_2)y+i(K_{3z}+K_{4z}-K_{1z}-K_{2z})z}\int dx\,e^{-(h/2\delta)[(x-\delta q_1/h)^2+(x-\delta q_2/h)^2+(x-\delta q_3/h)^2+(x-\delta q_4/h)^2]}$$

$$=\tfrac{1}{2}\beta\frac{1}{L_yL_z}\left(\frac{h}{2\pi\delta}\right)^{1/2}\delta_{q_1+q_2,q_3+q_4}\delta_{K_{1z}+K_{2z},K_{3z}+K_{4z}}e^{-(\delta/2h)[(q_1-q_3)^2+(q_2-q_3)^2]}\,.$$

Our final expression for the GL functional becomes

$$f=\sum_{K_z,q}(\alpha_H+\delta K_z^2)|\phi_{K_z,q}|^2+\frac{1}{2}\sum_{\substack{K_z,P_z,Q_z\\ k,p,q}}V(q,k-p)\phi^*_{K_z,k}\phi^*_{P_z+Q_z,p+q}\phi_{P_z,p}\phi_{K_z+Q_z,k+q}\,,\qquad(3.1)$$

where

$$V(q,k)=\beta'\exp\{-(\delta/2h)[q^2+k^2]\}\,,$$
$$\beta'=(\beta/L_yL_z)(h/2\pi\delta)^{1/2}\,.$$

To calculate the entropy it is convenient to introduce the fluctuation propagator

$$D(K_z)=\langle|\phi_{K_z,q}|^2\rangle=\int\prod_{K_z,q}(d^2\phi_{K_z,q})|\phi_{K_z,q}|^2e^{-f}\Big/\int\prod_{K_z,q}(d^2\phi_{K_z,q})e^{-f}\,.$$

From Eqs. (1.6) and (2.1) we have

$$S=-\int d^3r\langle|\psi(\vec{r})|^2\rangle=-\sum_{n,K_z,q}\langle|\phi_{n,K_z,q}|^2\rangle=-\sum_{K_z,q}D(K_z)\,,\qquad(3.2)$$

since we require the term $n=0$ only. $D(K_z)$ is given by the usual Feynman graph expansion.[12] Inclusion of only the Hartree self-energy essentially reproduces the results of Hassing, Hake, and Barnes.[9] Within the screening approximation[12] the propagator self-energy $\Sigma(K_z)$ and screened poten-

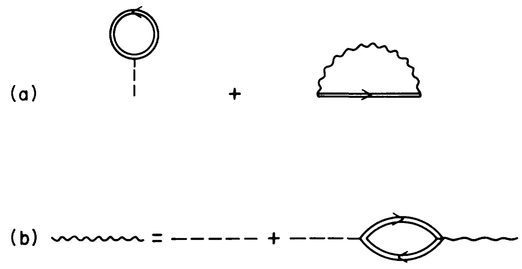

FIG. 1. (a) Diagrams for the propagator self-energy $\Sigma(K_z)$ within the screening approximation. A double bold line represents the dressed propagator and a wavy line the screened potential. (b) Diagrammatic equation for the screened potential.

tial $V_S(q, k, K_z)$ are given by the diagrams of Fig. 1. Note that the bare interaction potential $V(q, k)$ has a complicated momentum dependence so that the equations are not quite so simple as those of Ref. 12 where the bare potential is just a constant, namely, β/v. The analogs for our system of Eqs. (3) and (4) of Ref. 12 are

$$\Sigma(K_z) = \sum_{q', K_z'} V(0, q')D(K_z') + \sum_{q', K_z'} V_S(q', 0, K_z')D(K_z' + K_z) \tag{3.3}$$

and

$$V_S(q, k, K_z) = V(q, k) - E(K_z)\sum_{q'} V(q, q')\, V_S(q, k - q', K_z), \tag{3.4}$$

where

$$E(K_z) = \sum_{K_z'} D(K_z')D(K_z' + K_z)\ . \tag{3.5}$$

Equation (3.4) for $V_S(q, k, K_z)$ can be solved by Fourier transformation with respect to k. We first note that the bare potential $V(q, k)$ is factorizable:

$$V(q, k) = \beta' \exp[-(\delta/2h)(q^2 + k^2)] = v(q)v(k)\,,$$

where $v(q) = (\beta')^{1/2} e^{-\delta q^2/2h}$. Introduction of the Fourier transforms $V_S(q, x, K_z)$ and $v(x)$ through the relations

$$V_S(q, k, K_z) = \int_{-\infty}^{\infty} dx\, V_S(q, x, K_z)e^{ikx}\,,$$
$$v(k) = \int_{-\infty}^{\infty} dx\, v(x)e^{ikx}$$

yields, on substitution into Eq. (3.4),

$$V_S(q, x, K_z) = v(q)v(x) - \frac{E(K_z)}{2\pi} v(q) \sum_{q'} \int_{-\infty}^{\infty} dx\, e^{-ikx} \int_{-\infty}^{\infty} dx' v(x')e^{iq'x'}$$
$$\times \int_{-\infty}^{\infty} dx''\, V_S(q, x'', K_z)e^{i(k-q')x''} = v(q)v(x) - L_y E(K_z)v(q)v(x)\, V_S(q, x, K_z)\ .$$

Hence

$$V_S(q, x, K_z) = \frac{v(q)v(x)}{1 + L_y E(K_z)v(q)v(x)}\ . \tag{3.6}$$

To determine the self-energy $\Sigma(K_z)$ we require [from Eq. (3.3)]

$$\sum_q V_S(q, k=0, K_z) = \sum_q \int_{-\infty}^{\infty} dx\, V_S(q, x, K_z)$$
$$= \frac{1}{2\pi E(K_z)} \int\int_{-\infty}^{\infty} dx\, dq\, \frac{L_y E(K_z)v(q)v(x)}{1 + L_y E(K_z)v(q)v(x)}\ .$$

Substitution for $v(q)$ and $v(x)$ followed by integration over x and q yields

$$\sum_q V_S(q, k=0, K_z) = \frac{1}{E(K_z)} \ln\left(1 + \frac{\beta h}{2\pi\delta L_z} E(K_z)\right)\ .$$

In order to proceed further for the bulk case we are forced to approximate. An approximation which is both mathematically tractable and retains the essential features of the screening concept is to simply neglect the dependence of the screened potential on K_z. This involves replacing $V_S(q', 0, K_z')$ in Eq. (3.3) by $V_S(q', 0, 0)$. Using also $\sum_{q'} V(0, q') = \beta h/2\pi\delta L_z$, Eq. (3.3) becomes

$$\Sigma(K_z) = \frac{\beta h}{2\pi\delta L_z} \sum_{K_z'} D(K_z') + \frac{1}{E(0)} \ln\left(1 + \frac{\beta h}{2\pi\delta L_z} E(0)\right) \sum_{K_z'} D(K_z')\ .$$

The solution is of the form $D(K_z) = (\tilde{\alpha}_H + \delta K_z^2)^{-1}$, where

$$\tilde{\alpha}_H = \alpha_H + \frac{\beta h}{2\pi\delta L_z} \sum_{K_z} \frac{1}{\tilde{\alpha}_H + \delta K_z^2} + \frac{1}{E(0)} \ln\left(1 + \frac{\beta h E(0)}{2\pi\delta L_z}\right) \sum_{K_z} \frac{1}{\tilde{\alpha}_H + \delta K_z^2} \tag{3.7}$$

and, from Eq. (3.5),

$$E(0) = \sum_{K_z} \frac{1}{(\tilde{\alpha}_H + \delta K_z^2)^2}\ . \tag{3.8}$$

For the bulk case $\sum_{K_z} \to L_z \int_{-\infty}^{\infty} (dK_z/2\pi)$ and Eq. (3.8) gives $E(0) = L_z/(4\tilde{\alpha}_H[\tilde{\alpha}_H\delta]^{1/2})$. Substitution into Eq. (3.7) yields

$$\tilde{\alpha}_H = \alpha_H + \frac{\beta h}{2\pi\delta} \frac{1}{2(\tilde{\alpha}_H\delta)^{1/2}}$$

$$+2\tilde{\alpha}_H \ln\left(1+\frac{\beta h}{2\pi\delta}\,\frac{1}{4\tilde{\alpha}_H(\tilde{\alpha}_H\delta)^{1/2}}\right). \quad (3.9)$$

It is convenient for computational purposes to introduce dimensionless parameters x and y defined by

$$x=\frac{8\pi(\tilde{\alpha}_H\delta)^{3/2}}{\beta h}, \quad y=\alpha_H\delta\left(\frac{8\pi}{\beta h}\right)^{2/3}.$$

In terms of these, Eq. (3.9) becomes

$$y=x^{2/3}[1-2/x-2\ln(1+1/x)]. \quad (3.10)$$

The entropy is given by Eq. (3.2):

$$S=-\sum_{q,K_z} D(K_z)=-\sum_{q,K_z}\frac{1}{\tilde{\alpha}_H+\delta K_z^2}$$
$$=-\frac{eH}{\pi}L_xL_y\frac{L_z}{2(\tilde{\alpha}_H\delta)^{1/2}}=-\frac{veH}{2\pi(\tilde{\alpha}_H\delta)^{1/2}}.$$

The specific heat is therefore given by

$$C=\frac{dS}{d\alpha_H}=\frac{veH}{4\pi\tilde{\alpha}_H(\tilde{\alpha}_H\delta)^{1/2}}\,\frac{d\tilde{\alpha}_H}{d\alpha_H}=\frac{v}{\beta}\,\frac{1}{x}\,\frac{d\tilde{\alpha}_H}{d\alpha_H}.$$

Using Eq. (3.9), $d\tilde{\alpha}_H/d\alpha_H$ is obtained as

$$\frac{d\tilde{\alpha}_H}{d\alpha_H}=\left[1+\frac{1}{x}+\frac{3}{1+x}-2\ln\left(1+\frac{1}{x}\right)\right]^{-1}$$

giving

$$\frac{C}{\Delta C}=\frac{1+x}{1+5x+x^2-2x(1+x)\ln(1+1/x)}. \quad (3.11)$$

The specific heat is obtained as a function of $y=\alpha_H\delta(8\pi/\beta h)^{2/3}$ by numerically eliminating x between Eqs. (3.10) and (3.11). The result is plotted in Fig. 2. Also plotted is the Hartree approximation, derived from the following two equations which follow very simply from keeping only the first self-energy term of Fig. 1(a):

$$y=x^{2/3}(1-2/x), \quad C/\Delta C=(1+x)^{-1}.$$

The width of the transition is proportional to $H^{2/3}$ through the dependence of the temperature variable y on h. This result agrees with that of Lee and Shenoy,[2] based on free fluctuation theory: it is due in both cases to the inclusion of only the $n=0$ Landau orbital which should be a good approximation provided $\tilde{\alpha}_H \ll h$ since the energy of a fluctuation in the nth orbital is increased by $\sim 2nh$ relative to the case $n=0$ [see Eq. (2.2)]. The theory then contains the single dimensionless parameter $y=\alpha_H\delta(8\pi/\beta h)^{2/3}$ so that the $H^{2/3}$ scaling is independent of the particular approximation used to evaluate C. The peaking behavior exhibited in Fig. 2 is very similar to that obtained experimentally by Barnes and Hake,[8,9] and our theory reproduces the qualitative features of the transition curve much better than the Hartree theory used in Ref. 9. Detailed comparisons with experiment are not possible here since the experimental transition widths

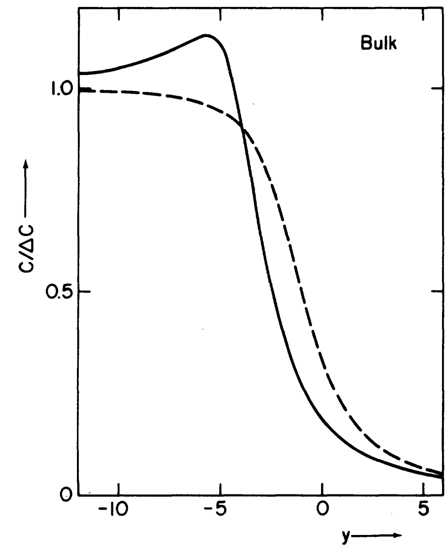

FIG. 2. Relative specific heat $C/\Delta C$ vs reduced relative temperature $y=\alpha_H\delta(8\pi/\beta h)^{2/3}$ for a bulk system. Continuous line: screening approximation; broken line: Hartree approximation.

are so large that our assumption (i) above breaks down. We will relax this assumption in Sec. IV in order to make such comparisons.

We turn now to the case of a thin superconducting film in a perpendicular magnetic field. The appropriate results are obtained from Eqs. (3.7) and (3.8) by suppressing the K_z degree of freedom. That is, we put $L_z=d$, the film thickness, and evaluate the sums by taking the terms $K_z=0$ only. This gives a fluctuation propagator $D=1/\tilde{\alpha}_H$, where

$$\tilde{\alpha}_H=\alpha_H+\frac{\beta h}{2\pi\delta d\tilde{\alpha}_H}+\tilde{\alpha}_H\ln\left(1+\frac{\beta h}{2\pi\delta d\tilde{\alpha}_H^2}\right). \quad (3.12)$$

Introducing dimensionless parameters x and y appropriate to the present case

$$x=\frac{2\pi\delta d\tilde{\alpha}_H^2}{\beta h}, \quad y=\alpha_H\left(\frac{2\pi\delta d}{\beta h}\right)^{1/2},$$

Eq. (3.12) becomes

$$y=x^{1/2}[1-1/x-\ln(1+1/x)]. \quad (3.13)$$

The specific heat is calculated in a manner analogous to the bulk case. The result is

$$\frac{C}{\Delta C}=\frac{1+x}{1+4x+x^2-x(1+x)\ln(1+1/x)}. \quad (3.14)$$

The specific heat is obtained as a function of $y=\alpha_H(2\pi\delta d/\beta h)^{1/2}$ by numerically eliminating x between Eqs. (3.13) and (3.14). The result is plotted in Fig. 3 together with the Hartree result, derived for the thin film case from the following two equations:

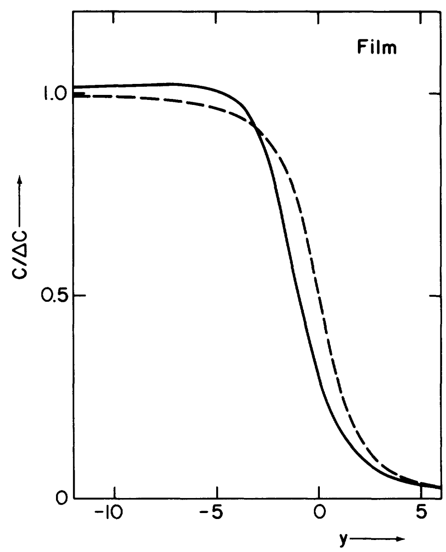

FIG. 3. Relative specific heat $C/\Delta C$ vs reduced relative temperature $y=\alpha_H(2\pi\delta d/\beta h)^{1/2}$ for a thin film. Continuous line: screening approximation; broken line: Hartree approximation.

$$y=x^{1/2}(1-1/x)\,,\quad C/\Delta C=(1+x)^{-1}\,.$$

The screening result for thin films is similar to that for the bulk case except that the peaking behavior is much less marked ($C/\Delta C$ has a maximum value of ~ 1.02 compared to ~ 1.13 for the bulk case.) For films the dimensionless parameter of the theory is $y=\alpha_H(2\pi\delta d/\beta h)^{1/2}$ so that the transition width scales as $H^{1/2}$.

IV. COMPARISON WITH EXPERIMENT

In this section we attempt to fit the prediction of the screening theory for bulk superconductors in a magnetic field to experimental data of Barnes and Hake[8] as reported in the paper of Hassing *et al.*[9] Measurements were made at six values of the magnetic field: $H=0$, 3, 8.8, 15, 22, and 29 kG. Our theory can only be expected to be valid for high enough fields ($h\gg\tilde{\alpha}_H$ must hold throughout the region of interest). For example the $H^{2/3}$ scaling of the transition width predicted by the theory clearly breaks down for small H, when the width tends to a constant. To obtain a rough guide to the region of validity of the theory we have estimated the experimental transition widths by measuring the maximum slope of the specific heat curves in the region where the specific heat is increasing rapidly. As expected we find that for small H the width tends to a constant while for large H it increases as a power of H. Our very rough estimate gives this power as ~ 0.8, compared to the theoretical value of $\frac{2}{3}$. The value of H at which the scaling behavior sets in is around 15 kG. We therefore restrict our comparisons of theory and experiment to the sets of data at 15, 22, and 29 kG.

Another important factor is that the experimental data covers a fairly wide temperature range (roughly 3–4 K for the sets of data we are considering). The assumption, therefore, that all the temperature dependence is contained in the parameter $\epsilon=(T-T_c)/T_c$ does not hold here. Instead we will use the form $\epsilon=\ln(T/T_0)$, where T_0 is the transition temperature in zero field, which follows from the microscopic derivation of the GL functional.[7] The standard form $\epsilon=(T-T_0)/T_0$ follows from an expansion about T_0. In addition we include the explicit temperature dependence in the relation $F=-T\ln Z_{\rm GL}$ and elsewhere; that is we do not set $T=T_c$ everywhere but include T explicitly. As a result we no longer obtain a one parameter solution. Finally, we note that $\xi_0/l\sim 100$ for the Ti-Mo alloy used by Barnes and Hake so that we can take the dirty limit where necessary.

Starting from the relation $F=-T\ln Z_{\rm GL}$ we obtain the entropy

$$S=\ln Z_{\rm GL}+T\,\frac{\partial\ln Z_{\rm GL}}{\partial T}\,. \tag{4.1}$$

Now

$$\alpha=\frac{\delta\epsilon}{\xi^2(0)}=\frac{1}{2mT\xi^2(0)}\ln\!\left(\frac{T}{T_0}\right)=\gamma\ln\!\left(\frac{T}{T_0}\right),$$

where $\gamma=3.84/k_F l$ in the dirty limit. Hence

$$\frac{d}{dT}=\frac{\gamma}{T}\,\frac{d}{d\alpha}\,.$$

(Strictly we should include derivatives with respect to δ and β in d/dT but these will give negligible contributions to S in the critical region.) Equation (4.1) becomes

$$S=\ln Z_{\rm GL}+\gamma\,\frac{\partial\ln Z_{\rm GL}}{\partial\alpha}\,,$$

giving

$$C=T\,\frac{\partial S}{\partial T}=\gamma\,\frac{\partial S}{\partial\alpha}=\gamma\,\frac{\partial\ln Z_{\rm GL}}{\partial\alpha}+\gamma^2\,\frac{\partial^2\ln Z_{\rm GL}}{\partial\alpha^2}\,. \tag{4.2}$$

Now

$$\frac{\partial\ln Z_{\rm GL}}{\partial\alpha}=-\sum_{q,K_z}\frac{1}{\tilde{\alpha}_H+\delta K_z^2}=-\frac{veH}{2\pi(\tilde{\alpha}_H\delta)^{1/2}}$$

and we have seen before in our one-parameter model that

$$\frac{\partial^2\ln Z_{\rm GL}}{\partial\alpha^2}=\frac{v}{\beta}f(x)\,,$$

where

$$f(x)=\frac{1+x}{1+5x+x^2-2x(1+x)\ln(1+1/x)}$$

and

$$x = 8\pi(\tilde{\alpha}_H\delta)^{3/2}/\beta h .$$

Equation (4.2) can therefore be written

$$C = \gamma^2 \frac{v}{\beta} f(x) - \gamma \frac{veH}{2\pi(\tilde{\alpha}_H\delta)^{1/2}} .$$

We normalize with respect to the mean-field jump at the transition in zero field

$$\Delta C = (\gamma^2 v/\beta)_{T=T_0} = 9.4\ N(0)T_0 .$$

Hence the normalized specific heat can be written

$$C/\Delta C = \frac{T}{T_0}\left(f(x) - \frac{\beta h}{4\pi\gamma\delta(\tilde{\alpha}_H\delta)^{1/2}}\right) = \frac{T}{T_0}[f(x) - \tfrac{1}{2}\lambda x^{-1/3}] ,$$

where

$$\lambda = [(8\pi)^{1/3}/2\pi\gamma\delta](\beta h)^{2/3} = \frac{1.22}{(k_F^2 l \xi_0)^{1/3}} h^{2/3} \text{ in the dirty limit.} = \kappa h^{2/3} .$$

Here κ is weakly temperature dependent through the dependence on $\xi_0 = 0.133 k_F/mT$. Hence we write

$$\kappa = \kappa_1 (T/T_0)^{1/3} ,$$

where κ_1 is defined by evaluating ξ_0 at $T = T_0$. We must also relate our field variable h to the measured field H. We have $h = 2e\delta H = eH/mT$. If H is measured in kG and T in kelvins this gives

$$h = 0.134 H/T .$$

Finally, we must relate our temperature variable y, given in terms of x by Eq. (3.10), to the real temperature T. From the definitions of λ and y we see that

$$\lambda y = 4\alpha_H/\gamma = 4\ln[T/T_c(H)] , \tag{4.3}$$

where $T_c(H)$ is the critical temperature T_{c2} given in the present model by the condition $\alpha_H = 0$. Equation (4.3) yields

$$T = T_{c2} e^{\lambda y/4} . \tag{4.4}$$

For convenience we collect together here the other equations of our solution

$$y = x^{2/3}[1 - 2/x - 2\ln(1 + 1/x)] , \tag{4.5}$$

$$\lambda = \kappa_1 (T/T_0)^{1/3}(0.134 H/T)^{2/3} , \tag{4.6}$$

$$C/\Delta C = (T/T_0)[f(x) - \tfrac{1}{2}\lambda x^{-1/3}] . \tag{4.7}$$

Equations (4.4)–(4.7) can be solved by numerically eliminating x and y to give $C/\Delta C$ as a function of T and H.

Since the simple GL functional (even our modified version) does not give the field dependence of $T_{c2}(H)$ correctly except for weak fields, we will regard $T_{c2}(15)$, $T_{c2}(22)$, and $T_{c2}(29)$ as adjustable parameters to be determined from the experimental results. Similarly, the expressions for the constants κ_1 and ΔC were derived on the basis of the free electron model of a metal—hardly a good approximation for the Ti-Mo alloy used by Barnes and Hake. We will therefore regard these too as adjustable parameters. The results are plotted as C versus T in Fig. 4. The following values of the parameters were used: $T_0 = 4.25$ K, $T_{c2}(15) = 3.82$ K, $T_{c2}(22) = 3.57$ K, $T_{c2}(29) = 3.30$ K, and $\kappa_1 = 0.036$; ΔC was chosen to give the correct peak height at 15 kG. Finally, the base line was lowered by 0.1 of a unit relative to that of Barnes and Hake in order to fit the high-temperature tail correctly. As given, the processed data points of Barnes and Hake actually run into the base line on the high-temperature side. This is in disagreement with all present theories[2,9,14] and may be due to a small error in the procedure used for subtracting out the specific heat of the normal state.[9]

V. DISCUSSION

The results depicted in Fig. 4 show that the screening theory predicts the shape of the transition very well—much better than the Hartree theory used by Hassing *et al.*[9] There is, however, still an inadequacy in the theory: it underestimates the amount by which the magnitude of the specific-heat jump falls off as the field H is increased. The reason for this inadequacy may lie in the breakdown of one or more of the assumptions made at the outset: the neglect of vortex-lattice structure, the inclusion of only the $n = 0$ Landau orbital and/or the use of the standard GL functional in strong magnetic fields. The last of these is certainly open to question: the microscopic derivation of the GL functional is only valid[5,6] provided $h \ll h_0 \sim \delta/\xi^2(0)$. Ref-

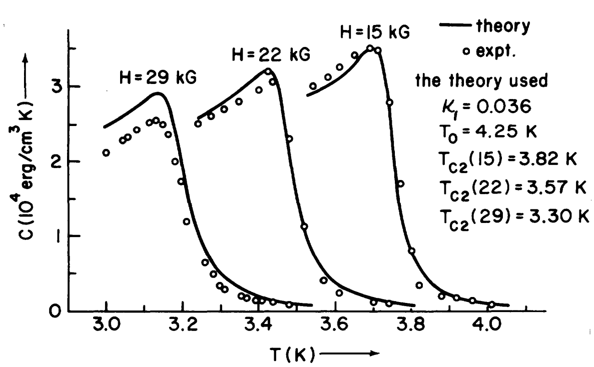

FIG. 4. Fluctuation specific heat C vs temperature T for various values of the applied magnetic field H. The open circles are the processed data of Barnes and Hake. The continuous curves represent the present theory.

erence 9 gives $\xi(0) \simeq 48\,\text{Å}$ which yields a maximum field $H_0 = h_0/2e\delta \sim 14$ kG, from which it is clear that high-field corrections to the GL functional are in principle required for the fields of Fig. 4.

If one performs a microscopic calculation to all orders in the field one finds[5,6] that the Gor'kov kernel (essentially the free fluctuation part of the GL functional) is still diagonalized by the Landau orbitals but that the eigenvalues are more complicated than the simple GL form. We only require the eigenvalues for the lowest orbital $n=0$. For small K_z we obtain a renormalization of δ, the coefficient of K_z^2 in the eigenvalue, together with a renormalization of α_H. The point to note is that neither of these renormalizations affects the value of the specific-heat jump. The second has already been accounted for by our choice of the T_{c2}'s to fit the data; the first gives a field dependent κ_1 which would affect the shape of the transition but not the specific-heat jump. The correct resolution of this problem remains an open question at the present time.

ACKNOWLEDGMENTS

I would like to thank the Science Research Council for financial support during the period when most of this work was performed. I am also indebted to the Fulbright-Hays Committee for a scholarship.

---

*Present address.

[1] A. J. Bray, Ph.D. thesis (University of Kent at Canterbury, 1973) (unpublished).
[2] P. A. Lee and S. R. Shenoy, Phys. Rev. Lett. 28, 1025 (1972).
[3] J. M. Ziman, *Principles of the Theory of Solids* (Cambridge U. P., Cambridge, England, 1964).
[4] L. G. Aslamazov and A. I. Larkin, Fiz. Tverd. Tela 10, 1104 (1968) [Sov. Phys.-Solid State 10, 875 (1968)].
[5] P. A. Lee and M. G. Payne, Phys. Rev. Lett. 26, 1537 (1971); Phys. Rev. B 5, 923 (1972).
[6] J. Kurkijarvi, V. Ambegaokar, and G. Eilenberger, Phys. Rev. B 5, 868 (1972).
[7] N. R. Werthamer, *Superconductivity*, edited by R. D. Parks (Marcel Dekker, New York, 1969), Vol. 1.
[8] L. J. Barnes and R. R. Hake, Phys. Rev. 153, 435 (1967).
[9] R. F. Hassing, R. R. Hake, and L. J. Barnes, Phys. Rev. Lett. 30, 6 (1973).
[10] S. Marcelja, Phys. Lett. A 28, 180 (1968); Phys. Rev. B 1, 2351 (1970); S. Marcelja, W. E. Masker, and R. D. Parks, Phys. Rev. Lett. 22, 124 (1969); Phys. Rev. 188, 745 (1969); L. Gunther and L. W. Gruenberg, Solid State Commun. 10, 567 (1972).
[11] S. Grossman, P. H. Richter, and C. Wissel, Solid State Commun. 11, 433 (1972).
[12] A. J. Bray and G. Rickayzen, J. Phys. F 2, L109 (1972).
[13] G. Rickayzen and A. J. Bray, J. Phys. F 3, L134 (1973).
[14] A. J. Bray, Phys. Lett. A 43, 277 (1973).