on $\Delta_s(r,t)$ which is zero above H_{cs}. This would result in an expression for D_d different from (3.21). It would be completely impossible to obtain anything close to H_{cs}. Near this field, the power expansion in $\Delta_d(r,t)$ would diverge. This would make impossible the derivations found in Sec. III.

To see how there is only one upper critical field for the two bands, we need only look at (2.3). We can interpret the energy gaps as resulting from pair correlation of electrons in both bands at the same time. Looking at the s-band energy gap, we can see that even at fields where the correlation of electrons in the s band is zero, the energy gap $\Delta_s(r,t)$ would not necessarily vanish. The d-band correlation would still exist. This is reminiscent of the continuing existence of the energy gaps above T_{cs} seen by Hafstrom *et al.* in the tunneling experiments on niobium.

[1]A. A. Abrikosov, Zh. Eksperim. i Teor. Fiz. 32, 1442 (1957) [Soviet Phys. JETP 5, 1174 (1957)].

[2]For a comprehensive review of experiments, see, for instance, Y. B. Kim and M. J. Stephen, in *Treatise on Superconductivity*, edited by R. D. Parks (Marcel Dekker, New York, 1968).

[3]M. J. Stephen and J. Bardeen, Phys. Rev. 140, A1197 (1965); M. Tinkham, Phys. Rev. Letters 13, 804 (1964); P. M. Anderson, N. R. Werthamer, and J. M. Luttinger, Phys. Rev. 138, A1157 (1965); P. G. de Gennes and P. Nozières, Phys. Letters 15, 216 (1965).

[4]A. Schmid, Physik Kondensierten Materie 5, 302 (1960).

[5]K. Maki and C. Caroli, Phys. Rev. 159, 306 (1967); 159, 316 (1967); 164, 591 (1967); K. Maki, *ibid.* 169, 381 (1968).

[6]T. Satoh and T. Ohtsuka, Phys. Letters 20, 565 (1966); H. A. Leupold and H. A. Boorse, Phys. Rev. 134, A1322 (1964); B. W. Maxfield and W. L. McLean, *ibid.* 139, A1515 (1965).

[7]H. Suhl, B. T. Matthias, and L. R. Walker, Phys. Rev. Letters 3, 552 (1959); J. Kondo, Progr. Theoret. Phys. (Kyoto) 29, 1 (1967).

[8]C. C. Sung and L. Yun Lung Shen, Phys. Letters 19, 101 (1965); V. Radhakrishnan, Phys. Status Solidi 20, 783 (1967).

[9]J. R. Carlson and C. B. Satterthwaite, Phys. Rev. Letters 24, 461 (1970).

[10]J. W. Hafstrom, R. M. Rose, and M. L. A. MacVicar, Phys. Letters 30A, 379 (1969).

[11]J. W. Garland, Jr., Phys. Rev. Letters 11, 111 (1963).

[12]I. Peschel, Solid State Commun. 4, 495 (1966).

[13]D. R. Tilley, Proc. Phys. Soc. (London) 84, 573 (1964).

[14]This condition occurs in superconducting niobium (see Ref. 18).

[15]L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, New York, 1962).

[16]A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Englewood Cliffs, N. J., 1963).

[17]This type of calculation is done by K. Maki, Phys. Rev. 164, 591 (1967).

[18]I. M. Tang, Phys. Letters 31A, 480 (1970).

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Theory of an Isolated Vortex in a Pure Superconductor near $T = T_c$*

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It is demonstrated that the theory of Bardeen, Kümmel, Jacobs, and Tewordt for an isolated vortex in a pure type-II superconductor at arbitrary temperatures is in agreement with the theory of Neumann and Tewordt near $T = T_c$ if nonanalytic terms of odd order in $(1 - T/T_c)^{1/2}$ in the free energy are assumed to vanish. The leading nonanalytic term is examined by the use of perturbation theory to see if it vanishes, but no definite conclusion can be drawn. The approximations used in deriving these results should prove useful in the application of the method of Bardeen *et al.* to other problems involving pure inhomogeneous superconductors.

I. INTRODUCTION

Bardeen *et al.*[1] (BKJT) have recently presented a theory for the properties of an isolated vortex in a pure type-II superconductor at arbitrary temperatures, thus giving a partial solution to one of the outstanding problems in type-II superconductivity.[2] Among other results, H_{c1} was obtained as a function of κ at 0 °K; an extension to higher temperatures is in progress.[3] The isolated vortex problem is also being treated by Eilenberger and Büttner who have recently published a preliminary report[4]; their theory is not limited to pure superconductors.

Prior to these efforts, the best theory for an isolated vortex was that of Neumann and Tewordt[5] who obtained the first-order correction term to the Ginzburg-Landau free energy[6] as derived by Gor'kov.[7] This theory is limited to the temperature region above about $0.9T_c$, but is valid for all values of κ and the mean free path.

Cleary[8] has recently demonstrated that the BKJT theory is in agreement with the Ginzburg-Landau-Gor'kov theory if a nonanalytic term of lower order in $(1 - T/T_c)$ is assumed to vanish. Since his proof does not test the correctness of a term in the BKJT free energy, it is important to reexamine the BKJT theory to see if it is in agreement with the Neumann-Tewordt theory.

In Sec. II, we review and reformulate the BKJT theory, and in Sec. III we obtain the leading terms in the expansion of the free energy near $T=T_c$. This expression is compared with the free-energy expression of Neumann and Tewordt in Sec. IV, and the two are shown to be identical if nonanalytic terms of odd order in $(1 - T/T_c)^{1/2}$ are assumed to vanish. In Sec. V, we consider the leading nonanalytic term, but are unable to show that it vanishes.

The reformulation of the BKJT theory in Sec. II, the high-energy expansion for the scattering states in Sec. III, and the perturbation expansion in Sec. V should be very useful in the application of the BKJT theory to other problems involving pure inhomogeneous superconductors.

II. REVIEW AND REFORMULATION OF BKJT THEORY

The expression of Bardeen *et al.*[1] for the Gibbs free energy of a pure superconductor containing a single vortex line is, relative to the Meissner state in the same applied field H_a,

$$\Delta G = \Delta G_m + \Delta G_a + \Delta G_b + \Delta G_{ci} , \tag{2.1}$$

where

$$\Delta G_m = \int d^2r\,(8\pi)^{-1}H^2(\vec{r}), \tag{2.2}$$

$$\Delta G_a = -\int d^2r(4\pi)^{-1}H(\vec{r})H_a = -H_a\hbar c/4e, \tag{2.3}$$

$$\Delta G_b = \pi\xi^2(0)N(0)\Delta_\infty^2(0)\tfrac{1}{2}\pi^2\int_0^\pi d\alpha\,\sin^3\alpha \times\int_0^\infty db\,(\tfrac{1}{2}\beta\Delta_\infty)^{-1}\ln\left(\frac{\cosh(\tfrac{1}{2}\beta\Delta_\infty)}{\cosh(\tfrac{1}{2}\beta\Delta_\infty\Lambda)}\right), \tag{2.4}$$

and

$$\Delta G_{ci} = \pi\xi^2(0)N(0)\Delta_\infty^2(0)\tfrac{1}{2}\pi\int_0^\pi d\alpha\,\sin^3\alpha\int_0^\infty db \times\int_1^{\hbar\omega_D/\Delta_\infty} d\Lambda[\Sigma(\Lambda, b, \alpha) - C(b, \alpha)(\Lambda^2-1)^{-1/2}]\tanh(\tfrac{1}{2}\beta\Delta_\infty\Lambda). \tag{2.5}$$

In these equations, H is the microscopic magnetic field; $\Delta_\infty = \Delta_\infty(T)$ is the BCS energy-gap parameter in wholly superconducting material at the temperature T; $\xi(T) = \hbar v_F/\pi\Delta_\infty(T)$; $N(0) = mp_F/2\pi^2$ is the one-spin density of states at the Fermi surface; $\alpha = \arccos(k_z/k_F)$; $b = \mu\Delta_\infty/E_F \sin^2\alpha$; k_z is the component of the wave number of the excitations parallel to the vortex line; and μ is related to the azimuthal quantum number of the excitations by Eq. (4.3) of Bardeen *et al.*[1] Equation (2.4) gives the contribution of the bound states to the free-energy difference, the energy eigenvalue E of the Bogoliubov equations being related to the quantity Λ by $E = \Lambda\Delta_\infty$. ΔG_{ci} as given by Eq. (2.5) is the sum of two terms, the contribution from the continuum states and the contribution from the interaction energy; the quantity Σ is the sum of the phase shifts of the continuum states with respect to the Meissner state, and

$$C(b, \alpha) = \lim \Lambda\Sigma(\Lambda, b, \alpha) \text{ as } \Lambda \to \infty . \tag{2.6}$$

Bardeen *et al.* have transformed the two second-order linear differential equations for $u(\vec{r})$ and $v(\vec{r})$ (the Bogoliubov equations) by means of the WKBJ approximation into two first-order nonlinear differential equations for the complex quantities η and ξ,

$$\frac{d\eta}{dx} + \delta(x)\cos\eta = \Lambda + F(x) , \tag{2.7}$$

$$\frac{2d\xi}{dx} = i\delta(x)\sin\eta , \tag{2.8}$$

where η and ξ are defined by Eqs. (4.3), (4.9), and (4.15) of Bardeen *et al.* The quantities x, δ, F, and Λ in Eqs. (2.7) and (2.8) are defined by

$$x = (2m\Delta_\infty/\hbar^2 k_\rho)(\rho^2 - \rho_t^2)^{1/2} , \tag{2.9}$$

$$\delta(x) = \Delta(\rho, T)/\Delta(\infty, T) , \tag{2.10}$$

$$F(x) = bq(x)/(b^2 + x^2) , \tag{2.11}$$

and

$$\Lambda = E/\Delta_\infty(T) . \tag{2.12}$$

The quantity $\rho_t = \mu/k_\rho$ is the turning point of the WKBJ approximation and the quantity $q(\rho)$ is related to the microscopic magnetic field $H(\rho)$ by

$$H(\rho) = -(\hbar c/2e)\rho^{-1}\frac{dq(\rho)}{d\rho}. \tag{2.13}$$

For the bound states, η is real and ξ is imaginary; the bound-state eigenvalue Λ is that value of Λ for which the boundary condition $\eta(x=0) = n\pi$, $n = 0, \pm 1, \pm 2, \ldots$, is satisfied. Note that there can be several branches to the bound-state spectrum corresponding to the various values of n. In practice, it is found that there are no branches to the spectrum for $n > 0$. Also, the branches for $n < 0$ appear only for small values of α; for the variational functions for $\delta(x)$ and $q(x)$ used by Bardeen *et al.*, a second branch (that for $n = -1$) occurred only in the case $a = c = 0.25$.

For the continuum states, both η and ξ are complex; $\eta = \eta_1 - i\eta_2$ and $\xi = \xi_1 - i\xi_2$. Because of the degeneracy described by Bardeen *et al.*, the boundary condition at $x=0$ is not an eigenvalue condition like that for the bound states, but instead, a condition on the value of ξ at $x=0$. There are two independent solutions given by

$$\sin[\xi_1^{\pm}(0)+\tfrac{1}{2}\eta_1(0)]=\pm e^{-\eta_2(0)}\sin[\xi_1^{\pm}(0)-\tfrac{1}{2}\eta_1(0)]$$

or (2.14)

$$\tan\xi_1^{\pm}(0)=-\tan\tfrac{1}{2}\eta_1(0)[\tanh\tfrac{1}{2}\eta_2(0)]^{\mp 1}\ .$$

In terms of $\xi_1^{\pm}(0)$, the total phase shift Σ is given by Bardeen *et al.*[1] as

$$\Sigma=\sigma(b>0)+\sigma(b<0)\ , \tag{2.15}$$

where

$$\sigma=\xi_1^{+}(0)+\xi_1^{-}(0)+\int_0^\infty dx[\delta(x)\cos\eta_1(x)\times\sinh\eta_2(x)-\sinh\eta_2(\infty)]\ . \tag{2.16}$$

We first note that Eq. (2.16) may be rewritten with the help of Eq. (2.7) as

$$\sigma=\arctan\{\tan\eta_1(0)[\tanh\eta_2(0)-1]/[\tanh\eta_2(0)+\tan^2\eta_1(0)]\}-\int_0^\infty dx[\delta(x)\cos\eta_1(x)e^{-\eta_2(x)}-e^{-\eta_2(\infty)}-F]\ . \tag{2.17}$$

The second step in simplifying the result of Bardeen *et al.* is to transform to a new variable w defined by

$$w=\exp(-i\eta)\ . \tag{2.18}$$

The differential equation for w is

$$2i\frac{dw}{dx}=-\delta(1+w^2)+2(\Lambda+F)w\ . \tag{2.19}$$

The expression for σ simplifies to

$$\sigma=\arctan\left(-\frac{2u(0)v(0)}{1-u^2(0)+v^2(0)}\right)-\int_0^\infty dx[\delta(x)u(x)-w(\infty)-F]$$
$$=-\int_0^\infty dx\left(\delta(x)u(x)-w(\infty)-F+\frac{d\arctan[-2uv/(1-u^2+v^2)]}{dx}\right)\ , \tag{2.20}$$

where the real and imaginary parts of w are given by

$$w=u-iv \tag{2.21}$$

and the value of w at $x=\infty$ is

$$w(\infty)=\exp[-\eta_2(\infty)]=\Lambda-(\Lambda^2-1)^{1/2}\ . \tag{2.22}$$

Equation (2.20) can be further simplified to

$$\sigma=\int_0^\infty dx\left[-\delta u+w(\infty)+F-2\,\mathrm{Im}\left(w(1-w^2)^{-1}\frac{dw}{dx}\right)\right]$$
$$=-\mathrm{Im}\log[1-w^2(0)]+\int_0^\infty dx[w(\infty)+F-\delta u]\ . \tag{2.23}$$

Another form for σ can be obtained by performing the differentiation in Eq. (2.20) and using the real and imaginary parts of Eq. (2.19) to remove the derivatives; the result is

$$\sigma=\int_0^\infty dx\{w(\infty)-2\Lambda-F+2\,\mathrm{Re}[(\Lambda+F-\delta w)/(1-w^2)]\}\ . \tag{2.24}$$

These results are preferable to the BKJT formulation for both analytic and numerical work involving the scattering states.

Bergk and Tewordt[9] have transformed Eq. (2.7) by means of the substitution

$$\zeta(x)=\tan\tfrac{1}{2}\eta(x)\ , \tag{2.25}$$

the differential equation for $\zeta(x)$ being

$$2\frac{d\zeta}{dx}=(\Lambda+F-\delta)+(\Lambda+F+\delta)\zeta^2\ . \tag{2.26}$$

The transformation (2.25) is preferable to both the BKJT formulation and Eq. (2.18) for calculations involving the bound states. The variables w and ζ are related by

$$i\zeta=(1-w)/(1+w)\ . \tag{2.27}$$

III. BKJT THEORY NEAR $T=T_c$

The results described in Sec. II are valid for all temperatures less than T_c; it is of great interest to compare the BKJT theory near $T=T_c$ with the well-known results of Ginzburg and Landau,[6] as modified by Gor'kov.[7] Cleary[8] has recently given an ingenious proof that the BKJT free energy is identical to the Ginzburg-Landau free energy to terms of order $(1-t)=(1-T/T_c)$, if the coefficient of a term of order $(1-t)^{1/2}$ in the BKJT free energy vanishes. He first notes that the contribution from the bound states (ΔG_b) can be expanded about $\Delta_\infty/2T=0$ in a power series in which only odd powers of $\Delta_\infty/2T$ occur; since Δ_∞ is proportional to $(1-t)^{1/2}$ near $t=1$, ΔG_b cannot contribute terms of integral powers of $(1-t)$. He then solves Eq. (2.7) in powers of Λ^{-1} so that the quantity

$$\Sigma(\Lambda,b,\alpha)-C(b,\alpha)/(\Lambda^2-1)^{1/2}$$

is obtained to the lowest nonvanishing order of Λ^{-1}; on integrating this term over Λ, he finds a term proportional to $(1-t)$. Finally, he shows that the coefficient of this term is identical to the coefficient of the corresponding term in the Ginzburg-Landau free energy.

Since Cleary's proof tests only the integral part of the phase shift Σ as defined by Eqs. (2.15) and (2.16) and not the $\xi^{\pm}(0)$ part, it is of interest to calculate the term of next higher order in $(1-t)$ in the BKJT free energy and to compare it with the corresponding term found by Neumann and Tewordt.[5]

Following Cleary's idea, we expand w in powers of Λ^{-1},

$$w=(u_1-iv_1)\Lambda^{-1}+(u_2-iv_2)\Lambda^{-2}+\cdots \, . \tag{3.1}$$

On inserting this expansion into Eq. (2.19) and equating the coefficients of Λ^{-n}, we find

$$\begin{aligned}
&u_1=\tfrac{1}{2}\delta\,, \qquad v_1=0\,,\\
&u_2=-\tfrac{1}{2}F\delta\,, \qquad v_2=-\tfrac{1}{2}\delta'\,,\\
&u_3=-\tfrac{1}{2}\delta''+\tfrac{1}{2}F^2\delta+\tfrac{1}{8}\delta^3\,,\ v_3=\tfrac{1}{2}F'\delta+F\delta'\,,\\
&u_4=-\tfrac{3}{8}F\delta^3-\tfrac{1}{2}F^3\delta+\tfrac{1}{2}F''\delta+\tfrac{3}{2}(F'\delta'+F\delta'')\,,\\
&v_4=\tfrac{1}{2}\delta'''-\tfrac{5}{8}\delta^2\delta'-\tfrac{3}{2}F(F'\delta+F\delta')\,,\\
&u_5=\tfrac{1}{2}\delta''''-\tfrac{1}{8}\delta[11(\delta')^2+7\delta\delta'']+\tfrac{1}{16}\delta^5+\tfrac{3}{4}F^2\delta^3+\tfrac{1}{2}F^4\delta\\
&\qquad -\tfrac{3}{2}\delta(F')^2-F(6F'\delta'+3F\delta''+2F''\delta)\,.
\end{aligned}\tag{3.2}$$

The above relations suffice to determine the $\delta(x)u(x)$ term in the integrand of Eq. (2.20) to terms of order Λ^{-5}. The expression for the arctan part can be derived from the following expression (correct to fifth order in Λ^{-1}):

$$\arctan[-2uv/(1-u^2+v^2)]=u_1v_2\Lambda^{-3}+(u_1v_3+u_2v_2)\Lambda^{-4}+(u_1v_4+u_2v_3+u_3v_2+u_1^3v_2)\Lambda^{-5}\,. \tag{3.3}$$

The terms in Λ^{-2} and Λ^{-4} are odd in F and cancel on calculating Σ; the result is

$$\begin{aligned}
\Sigma=-\int_0^\infty dx\{&\Lambda^{-1}(\delta^2-1)+\Lambda^{-3}[\tfrac{1}{4}(\delta^4-1)+F^2\delta^2+(\delta')^2]\\
&+\Lambda^{-5}[\tfrac{5}{2}(\delta\delta')^2+\tfrac{1}{8}(\delta^6-1)-2\delta'\delta'''+\tfrac{3}{2}F^2\delta^4-(\delta'')^2\\
&+F^4\delta^2+(\delta F')^2+8FF'\delta\delta'+6(F\delta')^2]\}\,.
\end{aligned}\tag{3.4}$$

The term in Σ of order Λ^{-1} was found first by Bergk and Tewordt,[9] and shows that

$$C(b,\alpha)=\int_0^\infty dx\,(1-\delta^2)\,. \tag{3.5}$$

The term of order Λ^{-3} was, of course, found by Cleary.[8]

The next step is to integrate Eq. (3.4) over b and to change variables from b and x to R and θ, where $x=R\cos\theta$ and $b=R\sin\theta$. After performing the integration over θ, we find

$$\begin{aligned}
\int_0^\infty db\,\Sigma=\tfrac{1}{2}\pi\int_0^\infty R\,dR\{&\Lambda^{-1}(1-\delta^2)\\
&+\tfrac{1}{2}\Lambda^{-3}[\tfrac{1}{2}(1-\delta^4)-v^2\delta^2-(\delta')^2]\\
&+\tfrac{1}{4}\Lambda^{-5}[\tfrac{1}{2}(1-\delta^6)-5(\delta\delta')^2-3\delta^4v^2-\tfrac{1}{2}W(R)]\\
&+\tfrac{1}{4}\Lambda^{-5}[3(\delta'')^2+5\delta'\delta''/R+3\delta'\delta'''-\delta\delta''v^2\\
&-(v\delta')^2-\delta\delta'v^2/R-2\delta\delta'vv']\}\,,
\end{aligned}\tag{3.6}$$

where the derivatives are now with respect to R and $v(R)=q(R)/R$; the quantity $W(R)$ is given by

$$W(R)=3(\delta''+\delta'/R-\delta v^2)^2-4\delta''(\delta'/R-\delta v^2)+(2\delta'v+\delta v'-\delta v/R)^2. \tag{3.7}$$

By several integrations by parts, it can be shown that the integral over the last square bracket in Eq. (3.6) is identically zero. We next subtract $C(\Lambda^2-1)^{-1/2}$ from Σ and integrate over α; on changing the variable of integration from R to $\rho=\frac{1}{2}\pi R\xi\sin\alpha$ and performing the α integral, we have

$$\begin{aligned}
\int_0^\pi \sin^3\alpha\,d\alpha\int_0^\infty db[\Sigma(\Lambda,b,\alpha)-C(b,\alpha)(\Lambda^2-1)^{-1/2}]&\\
=\int_0^\infty\rho\,d\rho\{-\pi6^{-1}\Lambda^{-3}[6\pi^{-2}\xi^{-2}(1-\delta^2)^2+2(\delta')^2+2\delta^2v^2]&\\
+\pi^3\xi^2 60^{-1}\Lambda^{-5}[30\pi^{-4}\xi^{-4}(-\delta^6+3\delta^2-2)&\\
-50\pi^{-2}\xi^{-2}(\delta\delta')^2-30\pi^{-2}\xi^{-2}\delta^4v^2-W(\rho)]\}&\,,
\end{aligned}\tag{3.8}$$

where the derivatives now are with respect to ρ and $v=q(\rho)/\rho$. The result (3.8) can now be substituted into Eq. (2.5); the necessary integrals over Λ are evaluated in the Appendix. The result for ΔG up to second order in $(1-t)$ according to the BKJT theory is

$$\begin{aligned}
\Delta G_{\mathrm{BKJT}}=\Delta G_m+\Delta G_a+\Delta G_b+\Delta G_0+\pi\xi^2(0)N(0)\Delta_\infty^2(0)&\\
\times\int_0^\infty\rho\,d\rho&\\
\times\{7\zeta(3)12^{-1}(\Delta_\infty/2T)^2[6\pi^{-2}\xi^{-2}(1-\delta^2)^2&\\
+2(\delta')^2+2\delta^2v^2]+31\zeta(5)120^{-1}\xi^2(\Delta_\infty/2T)^4&\\
\times[30\pi^{-4}\xi^{-4}(-\delta^6+3\delta^2-2)-50\pi^{-2}\xi^{-2}(\delta\delta')^2&\\
-30\pi^{-2}\xi^{-2}\delta^4v^2-W(\rho)]\}&\,,
\end{aligned}\tag{3.9}$$

where ΔG_0 represents terms of odd order in $(\Delta_\infty/2T)$ resulting from the integration over Λ.

Since we want the second term inside the curly bracket in Eq. (3.9) to only the lowest order, we can use

$$(\Delta_\infty/2T)^4=4\pi^4(1-t)^2/49\zeta^2(3)\,. \tag{3.10}$$

A better approximation, given below, is necessary for $(\Delta_\infty/2T)^2$.

Bergk and Tewordt[9] have also obtained a high-energy expansion for the phase shift by starting from Eq. (2.26) and making transformations of the independent and dependent variables according to the theory of the Riccati equation[10]; a linear second-order differential equation is obtained, which is solved by a WKBJ method. This expansion is clearly asymptotic and hence, the expansion (3.1) must also be asymptotic. As we shall prove in Sec. IV, the latter expansion gives the Neumann-Tewordt expression for the free energy of an isolated vortex and so expansions about $T=T_c$ are asymptotic. To the author's knowledge, this was first pointed out by Helfand and Werthamer.[11]

IV. COMPARISON WITH NEUMANN-TEWORDT RESULT

The expression for the free energy difference ΔG for a pure superconductor is,[5] in ordinary units,

$$\Delta G_{\rm NT}=\Delta G_m+\Delta G_a+\int_0^\infty\rho\,d\rho\{\tfrac14H_c^2(1-\delta^2)^2+H_c^2\lambda^2[(\delta')^2+\delta^2v^2]/2\kappa_3^2\}+(1-t)[93\zeta(5)H_c^2\lambda^4/490\zeta^2(3)\kappa_3^4]\int_0^\infty\rho\,d\rho$$
$$\times\{-5\kappa_3^4\delta^2(1-\delta^2)^2/6\lambda^4+5\kappa_3^2(1-\delta^2)[(\delta')^2+\delta^2v^2]/\lambda^2-10\kappa_3^2(\delta\delta')^2/3\lambda^2-W(\rho)\}\;, \qquad (4.1)$$

where λ is the penetration depth, $\kappa_3=2\sqrt2\,eH_c\lambda^2$ and $W(\rho)$ is given by Eq. (3.7) with R replaced by ρ. In the second integral, we need only the lowest-order terms in the expansion of H_c and λ/κ_3 in powers of $(1-t)$ and hence, we may set

$$H_c^2=H_c^2(0)8\gamma^2(1-t)^2/7\zeta(3)\;, \qquad (4.2)$$

and

$$\lambda^2/\kappa_3^2=\pi^2\xi^2/6\;. \qquad (4.3)$$

The Neumann-Tewordt (NT) result can then be written as

$$\Delta G_{\rm NT}=\Delta G_m+\Delta G_a+\int_0^\infty\rho\,d\rho\{\tfrac14H_c^2(1-\delta^2)^2+H_c^2\lambda^2[(\delta')^2+\delta^2v^2]/2\kappa_3^2\}+\pi\xi^2(0)N(0)\Delta_\infty^2(0)[\pi^4\xi^2(1-t)^2 31\zeta(5)/1470\zeta^2(3)]$$
$$\times\int_0^\infty\rho\,d\rho\{-30\pi^{-4}\xi^{-4}\delta^2(1-\delta^2)^2+30\pi^{-2}\xi^{-2}[(\delta')^2+\delta^2v^2]-50\pi^{-2}\xi^{-2}(\delta\delta')^2-30\pi^{-2}\xi^{-2}\delta^4v^2-W(\rho)\}\;. \qquad (4.4)$$

On subtracting the NT result from the BKJT result, we have, to second order in $(1-t)$,

$$\Delta G_{\rm BKJT}-\Delta G_{\rm NT}=\Delta G_b+\Delta G_0+\pi\xi^2(0)N(0)\Delta_\infty^2(0)\int_0^\infty\rho\,d\rho\,\{(1-\delta^2)^2[\tfrac12\pi^{-2}\xi^{-2}7\zeta(3)(\Delta_\infty/2T)^2-\tfrac14H_c^2/\pi\xi^2(0)N(0)\Delta_\infty^2(0)]$$
$$+[(\delta')^2+\delta^2v^2][\tfrac78\zeta(3)(\Delta_\infty/2T)^2-\tfrac12H_c^2\lambda^2\kappa_3^{-2}/\pi\xi^2(0)\,N(0)\Delta_\infty^2(0)]\}$$
$$-\pi\xi^2(0)N(0)\Delta_\infty^2(0)[31\pi^2\zeta(5)\,(1-t)^2/49\zeta^2(3)]\int_0^\infty\rho\,d\rho\,[2\pi^{-2}\xi^{-2}(1-\delta^2)^2+(\delta')^2+\delta^2v^2]\;. \qquad (4.5)$$

The remaining step is to expand the quantities H_c^2, $H_c^2\lambda^2\kappa_3^{-2}$ and $(\Delta_\infty/2T)^2$ in powers of $(1-t)$; the results are

$$(\Delta_\infty/2T)^2=2\pi^2(1-t)\{1+(1-t)[\tfrac12+93\zeta(5)/98\zeta^2(3)]\}/7\zeta(3), \qquad (4.6)$$

$$[\xi(T)/\xi(0)]^2=7\zeta(3)\{1+(1-t)[\tfrac32-93\zeta(5)/98\zeta^2(3)]\}/8\gamma^2(1-t), \qquad (4.7)$$

$$H_c^2=\pi\xi^2(0)N(0)\Delta_\infty^2(0)4(1-t)\xi^{-2}\{1+(1-t)[\tfrac12-31\zeta(5)/98\zeta^2(3)]\}, \qquad (4.8)$$

$$H_c^2\lambda^2/\kappa_3^2=\pi\xi^2(0)\,N(0)\Delta_\infty^2(0)2\pi^2(1-t)3^{-1}\{1+(1-t)\,[\tfrac12-93\zeta(5)/98\zeta^2(3)]\}\;. \qquad (4.9)$$

On using Eqs. (4.6), (4.8), and (4.9) in Eq. (4.5), we find, to second order in $(1-t)$,

$$\Delta G_{\rm BKJT}-\Delta G_{\rm NT}=\Delta G_b+\text{terms of odd order in }(\Delta_\infty/2T)\,. \qquad (4.10)$$

The terms nominally of order $(1-t)$ and $(1-t)^2$ cancel; since ΔG_b contains only terms of odd order in $\Delta_\infty/2T$ and since $\Delta_\infty/2T$ contains only terms of odd order in $(1-t)^{1/2}$, we see that the three leading terms in $\Delta G_{\rm BKJT}-\Delta G_{\rm NT}$ are of order $(1-t)^{1/2}$, $(1-t)^{3/2}$ and $(1-t)^{5/2}$. It is, however, well known from the work of Gor'kov[7] and Tewordt[12] that $\Delta G_{\rm NT}$ is exact up to and including terms of order $(1-t)^2$ and hence, the first two terms must vanish. A term corresponding to the third term has been found by Hu and Korenman[13] as an extension to the results of Saint-James and de Gennes[14] and Ebneth and Tewordt[15] for $H_{c3}(T)/H_{c2}(T)$ near $T=T_c$, and so it is possible that the third term does not vanish. It is, however, more likely that the free energy of an isolated vortex contains only analytic terms since the nonanalytic term found by Hu and Korenman is intimately associated with the presence of an external surface.[16]

Since δ and v in the expressions for $\Delta G_{\rm BKJT}$ and $\Delta G_{\rm NT}$ are temperature dependent, $\Delta G_{\rm BKJT}$ and $\Delta G_{\rm NT}$ contain terms of higher order than the second in $(1-t)$; it is satisfying that these higher-order terms also are identical in the two theories.

V. NONANALYTIC TERMS IN ΔG

The leading term in the expansion of ΔG is[8]

$$\Delta G^{(1)}=\pi\xi^2(0)N(0)\Delta_\infty^2(0)[\pi\Delta_\infty(T)/4T]\times\int_0^\pi d\alpha\sin^3\alpha\int_0^\infty db\,\{\tfrac12\pi[1-\Lambda^2(b)]+\int_1^\infty\Lambda\,d\Lambda[\Sigma(\Lambda,b,\alpha)-C(b,\alpha)(\Lambda^2-1)^{-1/2}]\}\,. \qquad (5.1)$$

This term, which is of order $(1-t)^{1/2}$, must vanish in order that the BKJT theory reproduce the Ginzburg-Landau free energy near $T=T_c$. An exact calculation of $\Delta G^{(1)}$ appears to require an exact calculation of the bound-state eigenvalue Λ and the scattering-state phase shift Σ for all values of the parameters, and so a complete analytic investigation of the vanishing of $\Delta G^{(1)}$ seems to be impossible. It is, however, possible to find excellent approximations for Λ and w for a range of b and α values, and one might hope to show that the integrand in Eq. (5.1) (i.e., the contents of the curly bracket) vanishes for these values of b and α; as we will see, this expectation is unfortunately not fulfilled.

One case where good approximations can be found is that region of (b, α) values where $(1-\delta(x))$ and $F(x)$ are small for all values of x; under these conditions, one expects that an expansion in powers of $1-\delta(x)$ and $F(x)$ should be possible. We will first investigate the bound-state contribution to the $\Delta G^{(1)}$ integrand and afterwards go on to the scattering state contribution.

For the bound states, we begin with the differential equation (2.26) for $\zeta=\tan\frac{1}{2}\eta$ and expand ζ as

$$\zeta=\zeta_0+\zeta_1+\zeta_2+\cdots, \qquad (5.2)$$

where

$$\zeta_0=[(1-\Lambda)/(1+\Lambda)]^{1/2}, \qquad (5.3)$$

ζ_1 is of first order in $f(x)=1-\delta(x)$ and $F(x)$, ζ_2 is of second order, etc. On substituting Eq. (5.2) into Eq. (2.26) and sorting the terms according to their order, we obtain differential equations for the ζ's:

$$\frac{d\zeta_1}{dx}=(\Lambda+1)\zeta_0\zeta_1+\frac{\Lambda f+F}{\Lambda+1}, \qquad (5.4)$$

$$\frac{d\zeta_2}{dx}=(\Lambda+1)\zeta_0\zeta_2+\tfrac{1}{2}(\Lambda+1)\zeta_1^2+(F-f)\zeta_0\zeta_2. \qquad (5.5)$$

The solutions of these equations are

$$\zeta_1(x)=-\int_x^\infty dx_1\,(\Lambda f_1+F_1)\,(\Lambda+1)^{-1}\times\exp[-(\Lambda+1)\zeta_0(x_1-x)], \qquad (5.6)$$

$$\zeta_2(x)=-\int_x^\infty dx_1\,[\tfrac{1}{2}(\Lambda+1)\zeta_1^2(x_1)+(F_1-f_1)\zeta_0\zeta_1(x_1)]\times\exp[-(\Lambda+1)\zeta_0(x_1-x)]. \qquad (5.7)$$

We have used the notation $f_1=f(x_1)$, $F_1=F(x_1)$.

The bound-state eigenvalue Λ is obtained by setting $\zeta(x=0)$ equal to zero; for values of α which are not too small, the other branches of the bound-state spectrum do not appear. To second order, we have

$$(\Lambda+1)\zeta_0=J_1+J_2, \qquad (5.8)$$

where

$$J_1=\int_0^\infty dx_1(\Lambda f_1+F_1)\exp[-(\Lambda+1)\zeta_0x_1] \qquad (5.9)$$

and

$$J_2=\int_0^\infty dx_1[\tfrac{1}{2}(\Lambda+1)^2\zeta_1^2(x_1)+(\Lambda+1)(F_1-f_1)\zeta_0\zeta_1(x_1)]\times\exp[-(\Lambda+1)\zeta_0x_1]. \qquad (5.10)$$

On squaring Eq. (5.8) we obtain, to third order,

$$1-\Lambda^2=J_1^2+2J_1J_2. \qquad (5.11)$$

Since

$$(\Lambda+1)\xi_0=\int_0^\infty dx(f+F)+\text{second-order terms}$$

and

$$\Lambda=1+\text{second-order terms},$$

we may set $\Lambda=1$ and $(\Lambda+1)\zeta_0=0$ in Eq. (5.10) for J_2 and $\Lambda=1$ in Eq. (5.9) for J_1. The result for $1-\Lambda^2$, to third order in f and F, is

$$1-\Lambda^2=\left(\int_0^\infty dx_1g_1\right)^2-2\int_0^\infty dx_1\int_0^\infty dx_2\int_0^\infty dx_3x_2g_1g_2g_3+\int_0^\infty dx\int_0^\infty dx_1\int_x^\infty dx_2\int_x^\infty dx_3\,g_1g_2g_3, \qquad (5.12)$$

where

$$g(x)=f(x)+F(x),$$

On simplifying the above result, we find

$$1-\Lambda^2=\left[\int_0^\infty dx_1g_1\right]^2-2\int_0^\infty dx_1\int_0^\infty dx_3\int_{x_3}^\infty dx_2x_2g_1g_2g_3, \qquad (5.13)$$

correct to third order in f and F. The second-order term in Eq. (5.13) had been found previously by Cleary.[8]

For the scattering states, we expand w as

$$w=w_0+w_1+w_2+\cdots, \qquad (5.14)$$

where

$$w_0=\Lambda-(\Lambda^2-1)^{1/2}, \qquad (5.15)$$

w_1 is of first order in f and F, etc.; on inserting Eq. (5.14) into Eq. (2.19), sorting terms, and solving the resulting differential equations, we find[17]

$$w_1(x)=iw_0\int_x^\infty dx_1(\Lambda f_1+F_1)\exp[i(x_1-x)u] \qquad (5.16)$$

and

$$w_2(x)=-\tfrac{1}{2}w_1^2(x)/u-w_0u^{-1}\int_x^\infty dx_1\int_x^\infty dx_2\,(f_1+\Lambda F_1)\times(\Lambda f_2+F_2)\exp[i(x_2-x)u]. \qquad (5.17)$$

We have used the shorthand

$$u=(\Lambda^2-1)^{1/2}. \qquad (5.18)$$

Unfortunately, it is not possible to obtain a perturbation expansion for the quantity $(\Lambda+F-\delta w)/(1-w^2)$ in Eq. (2.24) which is valid for all values of Λ, and so it has not been possible to calculate the scattering-state contribution to the integrand of Eq. (5.1). If a perturbation expansion is possible after integrating over Λ, however, it is unlikely that odd powers of F will occur since the phase shift for $b<0$ is added to that for $b>0$. As we have seen, a perturbation expansion is possible for the bound-state contribution, and this expansion contains terms in odd powers of F. We conclude that it is unlikely that $\Delta G^{(1)}$ vanishes through the vanishing of the integrand for arbitrary δ and F. This conclusion can also be drawn without the use of perturbation theory; if one chooses δ and F to be constants for $x<X$ and $\delta=1$, $F=0$ for $x>X$, the differential equations can be solved exactly and a nonzero result for the $\Delta G^{(1)}$ integrand is obtained.

The condition that $\Delta G^{(1)}$ vanish for arbitrary δ and q may, however, be unnecessarily stringent; it is sufficient to require that $\Delta G^{(1)}$ vanish only for the exact functions δ and q (i.e., the functions which minimize the free energy). Since the exact δ and q are temperature dependent, $\Delta G^{(1)}$ as defined above contains terms of higher order than $(1-t)^{1/2}$; it is therefore sufficient to demand that $\Delta G^{(1)}$ vanish for the lowest-order [in $(1-t)$] exact functions – the solutions of the Ginzburg-Landau equations. One might therefore hope that the integrand of Eq. (5.1) can be rewritten in the form of integrals over the Ginzburg-Landau equations, but this appears to be impossible because the arguments of the various functions are not the same.

No progress has been made in the investigation of the next nonanalytic term in ΔG, $\Delta G^{(3)}$, and so the vanishing of this term in the BKJT theory is an open question.

The results of the perturbation theory used in this section are consistent with those obtained by Bardeen *et al.* from converting the differential equation (2.7) for η into an integral equation and iterating the result. The BKJT procedure gives more concise results but the expressions for ζ and w are not separated according to the powers of $(1-\delta)$ and F.

APPENDIX: EVALUATION OF INTEGRALS OVER Λ

In the derivation of Eq. (3.9) from Eq. (3.8), it is necessary to evaluate the integrals

$$I_1=\int_1^\infty d\Lambda\,\Lambda^{-3}\tanh(\Lambda\Delta_\infty/2T) \tag{A1}$$

and

$$I_2=\int_1^\infty d\Lambda\,\Lambda^{-5}\tanh(\Lambda\Delta_\infty/2T)\;. \tag{A2}$$

We have replaced the upper limits of the integrals by infinity since the integrals converge and we are interested in the weak coupling limit.

We first calculate I_1 which can be rewritten as

$$I_1=(\Delta_\infty/2T)\int_1^\infty d\Lambda\,\Lambda^{-2}-\int_0^1 d\Lambda\,\Lambda^{-3}\left(\tanh\frac{\Lambda\Delta_\infty}{2T}-\frac{\Lambda\Delta_\infty}{2T}\right)+\int_0^\infty d\Lambda\,\Lambda^{-3}\left(\tanh\frac{\Lambda\Delta_\infty}{2T}-\frac{\Lambda\Delta_\infty}{2T}\right)\;. \tag{A3}$$

The first integral is trivial, the second may be evaluated near $T=T_c$ (the exact condition is $|\Delta_\infty/\pi T|\leq 1$) by expanding the hyperbolic tangent in a power series and integrating term by term, and the third can be evaluated as a contour integral, the only singularities lying along the imaginary axis. The result is

$$I_1=\frac{\Delta_\infty}{2T}-\sum_{n=2}^\infty\frac{4(-1)^{n-1}}{(2n-3)\pi}\left(\frac{\Delta_\infty}{\pi T}\right)^{2n-1}\left(1-\frac{1}{2^{2n}}\right)\zeta(2n)-\frac{7\zeta(3)}{\pi^2}\frac{\Delta_\infty}{2T}\left|\frac{\Delta_\infty}{2T}\right|\;. \tag{A4}$$

Similarly, the result for I_2 is

$$I_2=\frac{1}{3}\frac{\Delta_\infty}{2T}-\frac{1}{3}\left(\frac{\Delta_\infty}{2T}\right)^3+\frac{31\zeta(5)}{\pi^4}\left(\frac{\Delta_\infty}{2T}\right)^3\left|\frac{\Delta_\infty}{2T}\right|-\sum_{n=3}^\infty\frac{4(-1)^{n-1}}{(2n-5)\pi}\times\left(\frac{\Delta_\infty}{\pi T}\right)^{2n-1}\left(1-\frac{1}{2^{2n}}\right)\zeta(2n)\;. \tag{A5}$$

It is remarkable that although I_1 and I_2 are odd functions of $\Delta_\infty/2T$, leading at first glance to the conclusion that ΔG_{ci} contains only odd powers of $(1-t)^{1/2}$, there are terms involving even powers of $(1-t)^{1/2}$, nevertheless.

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[1]J. Bardeen, R. Kümmel, A. E. Jacobs, and L. Tewordt, Phys. Rev. 187, 556 (1969).

[2]A. L. Fetter and P. C. Hohenberg, in *Treatise on Superconductivity*, edited by R. D. Parks (Marcel Dekker, New York, 1969), Chap. 15.

[3]A. E. Jacobs (unpublished).

[4]G. Eilenberger and H. Büttner, Z. Physik 224, 335 (1969).

[5]L. Neumann and L. Tewordt, Z. Physik 189, 55 (1966).

[6]V. L. Ginzburg and L. D. Landau, Zh. Eksperim. i Teor. Fiz. 20, 1064 (1950).

[7]L. P. Gor'kov, Zh. Eksperim. i Teor. Fiz. 36, 1918 (1959) [Soviet Phys. JETP 9, 1364 (1959)].

[8]R. M. Cleary, Phys. Rev. B 1, 1039 (1970).

[9]W. Bergk and L. Tewordt, Z. Physik 230, 178 (1970).

[10]E. L. Ince, *Ordinary Differential Equations* (Dover, New York, 1956).

[11]E. Helfand and N. R. Werthamer, Phys. Rev. 147, 288 (1966).

[12]L. Tewordt, Z. Physik 180, 385 (1964); Phys. Rev. 137, A1745 (1965).

[13]C.-R. Hu and V. Korenman, Phys. Rev. 185, 672 (1969).

[14]D. Saint-James and P.-G. de Gennes, Phys. Letters 7, 306 (1963).

[15]G. Ebneth and L. Tewordt, Z. Physik 185, 421 (1965).

[16]C.-R. Hu (private communication).

[17]These expressions, together with the expressions for the higher-order terms which have not been written down, can be used to derive the high-energy expansion of Sec. III, Eqs. (3.1) and (3.2); one merely uses the exponential terms in Eqs. (5.16), (5.17), etc., to perform repeated integrations by parts. This procedure usually results in asymptotic series, and thus one has further evidence that the high-energy expansion is only asymptotic.