impedance based on the wave functions and density of states of the Pincus surface states.

Garfunkel's simple model of a $\hbar\mathbf{k}_F\cdot\mathbf{v}_s$ energy shift, as we have shown can account equally well for the important frequency-temperature scaling of the data. But it is most certainly a much oversimplified description, especially in view of what is known about electron surface states in normal metals. The calculation based on cylindrical Fermi surface geometry and the $\hbar\mathbf{k}_F\cdot\mathbf{v}_s$ shift reproduces the derivative peak features, but falls short of detailed agreement with the experiments.

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Bardeen-Kümmel-Jacobs-Tewordt Theory of a Vortex near T_c†

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An expression for the free energy of a superconductor containing magnetic flux is derived for temperatures near T_c. To order T_c-T, the result is identical to that of Ginzburg-Landau as derived by Gor'kov. A term proportional to $(T_c-T)^{1/2}$ is shown to vanish in perturbation theory. The validity of the variational functions of Bardeen *et al.* is verified near T_c where the critical value of κ is almost identical to $1/\sqrt{2}$.

I. INTRODUCTION

It has been shown by Bardeen, Kümmel, Jacobs, and Tewordt how a variational calculation for the free energy of a superconductor containing magnetic flux may be performed.[1] They begin with a variational principle of Eilenberger.[2] Two trial functions for the order parameter and magnetic flux are taken for a superconductor containing a vortex and the result is minimized with respect to a parameter d for the order parameter and s for the magnetic flux. The variational functions of Ref. 1 are $\Delta(r)=\Delta_\infty\tanh(dr/\xi)$ and $(e/c)A(r)=\cosh(sr/\xi)/(2r)$, where $\xi=p_F/m\pi\Delta_\infty$ is the temperature-dependent coherence length, and Δ_∞ is the order parameter far from the vortex core in a gauge where $\Delta(r)$ is real. This calculation provides the variational values of s and d for a given κ, the Ginzburg-Landau (GL) parameter, and also the lower critical field H_{c1} may be derived as a function of κ by equating the vortex-state free energy to that of a superconductor in the Meissner state.[3] These calculations have been performed at 0 deg and can be extended to finite temperatures. Here we examine the free energy of a superconductor containing a vortex at temperatures near T_c. We assume that the free energy per unit length of vortex vanishes as $1-T/T_c$ as Gor'kov and Eilenberger have shown.[2,4]

The coefficient of $1-T/T_c$ is exactly proportional to the GL free energy. There is also a term of order $(1-T/T_c)^{1/2}$ which should vanish identically for any given smooth variational functions. We are only able to show that it vanishes in lowest-order perturbation theory at this time. Numerical calculations indicate that this term does indeed vanish.[5]

In Sec. II we summarize some of the basic equations of Bardeen *et al.* and proceed to isolate the free-energy terms to order $(1-T/T_c)^{1/2}$ and $1-T/T_c$. The coefficient of the linear term is calculated explicitly and is shown to be proportional to the GL free energy.

In Sec. III it is shown that the leading term in the temperature expansion will vanish identically in lowest-order perturbation theory for arbitrary, analytic, variational functions. This is unsatisfactory and it should be shown that the term vanishes for large variational functions. In Sec. IV the variational functions of Bardeen *et al.* are employed to calculate $H_{c1}(\kappa)$ using the GL free energy. The value of κ_c, the critical GL parameter separating type-I from type-II behavior is close to $1/\sqrt{2}$.

II. FREE ENERGY

The free energy of a superconductor may be derived from the expression[1]

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$$G_s=-2T\sum_n \ln[2\cosh(E_n/2T)]$$
$$+V^{-1}\int|\Delta(r)|^2d^3x+(8\pi)^{-1}\int(H(r)-H_a)^2d^3x, \quad (1)$$

where E_n are the energy eigenvalues ($E_n>0$) of the Bogoliubov equations.[6] V is the superconducting interaction parameter, $H(r)$ the magnetic field of the vortex, and H_a the externally applied field.

To obtain rapid convergence of the sum over n, one may calculate the free-energy difference with the Meissner state

$$\Delta G_s=-2T\sum_n \ln[(\cosh E_n/2T)/(\cosh E_n'/2T)]$$
$$+V^{-1}\int[|\Delta(r)|^2-\Delta_\infty^2]d^3x$$
$$+(8\pi)^{-1}\int H^2(r)d^3x-(c/4e)H_aL, \quad (2)$$

where E_n and E_n' are the energy eigenvalues for a superconductor containing a vortex and for one in the Meissner state.

The WKBJ approach reduces the two coupled second-order Bogoliubov equations to two first-order ones. The bound-state spectrum and scattering solutions contribute to ΔG in the following way:

$$\Delta G_s=-(L\pi\xi^2)N(0)\Delta_\infty^2\pi^2\frac{1}{2}\int_0^\pi d\alpha\,\sin^3\alpha\int_0^\infty db$$
$$\times\sum_i(2T/\Delta_\infty)\ln[(\cosh E_i(b)/2T)/(\cosh\Delta_\infty/2T)]$$
$$+(L\pi\xi^2)N(0)\Delta_\infty^2\pi\frac{1}{2}\int_0^\pi d\alpha\,\sin^3\alpha\int_0^\infty db\int_1^\infty d\lambda$$
$$\times[\Sigma(\lambda,b)-C(b)(\lambda^2-1)^{-1/2}]$$
$$\times\tanh(\lambda\Delta_\infty/2T)+\Delta G_m, \quad (3)$$

where

$$C(b)=\lim_{\lambda\to\infty}\lambda\Sigma(\lambda,b),$$

and ΔG_m is the contribution of the magnetic field to ΔG_s. $E_i(b)$ is the ith branch of the bound state spectrum and λ is the reduced energy E/Δ_∞ of the scattering states. b is related to the magnetic quantum number, and α is the angle of the trajectory of the excitations with the z axis. L is the length of vortex. Bergk has shown that the term in $C(b)$ exactly cancels $V^{-1}\int[|\Delta(r)|^2-\Delta_\infty^2]d^3x$.[1,7]

Expanding ΔG_s in terms of order

$$(\Delta_\infty/2T)\sim(1-T/T_c)^{1/2},$$

we have

$$\Delta G^{(1)}=(L\pi\xi^2)N(0)\Delta_\infty^2\pi\tfrac{1}{2}(\Delta_\infty/2T)\int_0^\pi d\alpha\,\sin^3\alpha$$
$$\times\int_0^\infty db\left\{\tfrac{1}{2}\pi[1-\lambda^2(b)]\right.$$
$$\left.+\int_1^\infty\lambda d\lambda[\Sigma(\lambda,b)-C(b)(\lambda^2-1)^{-1/2}]\right\}. \quad (4)$$

From previous work by Gor'kov and Eilenberger,[2,4] we are to believe that this term vanishes. The lowest nonvanishing term should be of order $(\Delta_\infty/2T)^2\sim(1-T/T_c)$. ΔG_m is of this order and ΔG_b, the bound-state contribution, only gives terms of order $(\Delta_\infty/2T)^{n/2}$, where n is an odd integer. The term we seek must be obtained from the scattering-state contribution.

If one expands

$$\Sigma(\lambda,b)=C(b)/\lambda+D(b)/\lambda^3+O(1/\lambda^5), \quad (5)$$
$$C(b)/(\lambda^2-1)^{1/2}=C(b)/\lambda+C(b)/2\lambda^3+O(1/\lambda^5), \quad (6)$$

the only term which can contribute to order $(\Delta_\infty/2T)^2$ is proportional to $[D(b)-C(b)/2]\lambda^{-3}$. For example, the term $O(1/\lambda^5)$ only contributes to $(\Delta_\infty/2T)^4$ in even powers. We have

$$\int_1^\infty\frac{d\lambda}{\lambda^3}\tanh\frac{\lambda\Delta_\infty}{2T}$$
$$=\frac{\Delta_\infty}{2T}-\left(\frac{\Delta_\infty}{2T}\right)^2\int_0^\infty\frac{d\lambda}{\lambda}\frac{\tanh\lambda}{\cosh^2\lambda}+0\left(\frac{\Delta_\infty}{2T}\right)^3. \quad (7)$$

Therefore the leading term as $T\to T_c$ is

$$\Delta G_s^{(2)}=-(L\pi\xi^2)N(0)\Delta_\infty^2\tfrac{1}{2}\pi\left(\frac{\Delta_\infty}{2T}\right)^2\int_0^\infty\frac{d\lambda}{\lambda}\frac{\tanh\lambda}{\cosh^2\lambda}$$
$$\times\int_0^\pi d\alpha\,\sin^3\alpha\int_0^\infty db[D(b)-\tfrac{1}{2}C(b)]$$
$$+\frac{1}{8\pi}\int H^2(r)d^3r-\frac{c}{4e}H_aL. \quad (8)$$

We now solve for $\Sigma(\lambda,b)$ to order λ^{-3} using the WKBJ equations,

$$\frac{d\omega_1}{dx}+\delta(x)\cos\omega_1\cosh\omega_2=\lambda+F(x), \quad (9)$$

$$\frac{d\omega_2}{dx}=\delta(x)\sin\omega_1\sinh\omega_2. \quad (10)$$

Here x is defined by $r/\xi=(\pi/2)\sin\alpha(x^2+b^2)^{1/2}$ and $\delta(x)=\Delta(x)/\Delta_\infty$. $F(x)$ is given by $bq(x)/(b^2+x^2)$ with $q(r)=2erA(r)/c$, and $A(r)$ is the magnetic vector po-

[6] N. N. Bogoliubov, V. V. Tolmachev, and D. V. Shirkov, *A New Method in the Theory of Superconductivity* (Consultants Bureau, Inc., New York, 1959).
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tential. Writing

$$\omega_1=\frac{a}{\lambda+F}+\frac{b}{(\lambda+F)^2}+\cdots, \tag{11}$$

$$\operatorname{sech}\omega_2=\frac{A}{\lambda+F}+\frac{B}{(\lambda+F)^2}+\frac{C}{(\lambda+F)^3}+\cdots, \tag{12}$$

one may easily verify by direct substitution that

$$a=-\delta'/\delta,\quad A=\delta, \tag{13}$$

$$B=0,\qquad C=-\delta''+\tfrac{1}{2}\delta'^2/\delta. \tag{14}$$

These are the only terms needed to calculate $C(b)$ and $D(b)$.

The function $\Sigma(\lambda,b)$ is defined as follows:

$$\Sigma(b)=\sigma(b)+\sigma(-b), \tag{15}$$

where

$$\sigma(\pm b)=\xi_1^{(+)}(0)^{\pm}+\xi_1^{(-)}(0)^{\pm}+\int_0^\infty dx \times[\delta(x)\cos\omega_1^{\pm}(x)\sinh\omega_2^{\pm}(x)-\sinh\omega_2(\infty)], \tag{16}$$

and

$$\xi_1^{\pm}(0)=-\tan^{-1}\left\{\tan\frac{\omega_1^{(0)}}{2}\left[\tanh\frac{\omega_2^{(0)}}{2}\right]^{\mp1}\right\}. \tag{17}$$

Using

$$\sinh\omega_2(\infty)=\lambda-\frac{1}{2\lambda}-\frac{1}{8\lambda^3}+\cdots$$

one may show that

$$\begin{aligned}\Sigma(\lambda,b)=&\,\xi_1^{+}(0)^{+}+\xi_1^{+}(0)^{-}+\xi_1^{-}(0)^{+}+\xi_1^{-}(0)^{-}\\&+\omega_1^{+}(0)+\omega_1^{-}(0)+\int_0^\infty dx\Big\{-\delta(x)\cos\omega_1^{+}(x)\\&\times[\tfrac{1}{2}\operatorname{sech}\omega_2^{+}(x)+\tfrac{1}{8}\operatorname{sech}^3\omega_2^{+}(x)]\\&-\delta(x)\cos\omega_1^{-}(x)[\tfrac{1}{2}\operatorname{sech}\omega_2^{-}(x)+\tfrac{1}{8}\operatorname{sech}^3\omega_2^{-}(x)]\\&+\frac{1}{\lambda}+\frac{1}{4\lambda^3}\Big\}+0\left(\frac{1}{\lambda^4}\right).\end{aligned} \tag{18}$$

A simple calculation will demonstrate that

$$\xi^{+}(0)^{+}+\xi^{+}(0)^{-}+\xi^{-}(0)^{+}+\xi^{-}(0)^{-}+\omega_1^{+}(0)+\omega_1^{-}(0)=\delta'(0)\delta(0)/\lambda^3+0(1/\lambda^4). \tag{19}$$

But $\delta'(0)=0$, if $b\neq0$. We have therefore

$$C(b)=\int_0^\infty dx(1-\delta^2), \tag{20}$$

and

$$D(b)=\int_0^\infty dx[\tfrac{1}{4}(1-\delta^4)-F^2\delta^2-\delta'^2+\tfrac{1}{2}(\delta^2)'']. \tag{21}$$

Equation (20) was first derived by Bergk.[1,7] The term proportional to $(\delta^2)''$ is identically zero as one may verify by straightforward integration.

The tabulated integral

$$\int_0^\infty\frac{d\lambda}{\lambda}\frac{\tanh\lambda}{\cosh^2\lambda}=\frac{7\zeta(3)}{\pi^2}$$

simplifies the expression for $\Delta G_s^{(2)}$, which becomes

$$\begin{aligned}\Delta G_s^{(2)}=&-(L\pi\xi^2)N(0)\Delta_\infty^2\pi\tfrac{1}{4}(\Delta_\infty/2T)^2\\&\times7\zeta(3)\pi^{-2}\int_0^\pi d\alpha\sin^3\alpha\int_0^\infty db\int_0^\infty dx\\&\times[\delta^2-1+\tfrac{1}{2}(1-\delta^4)-2F^2\delta^2-2\delta'^2]\\&+(8\pi)^{-1}\int H^2d^3x-(c/4e)H_aL.\end{aligned} \tag{22}$$

The order parameter δ is a function of (x^2+b^2) and the integration over b and x can be converted to one over the radial coordinate r. We have finally

$$\begin{aligned}\Delta G_s^{(2)}=&\,2\pi L|\Psi_0|^2\int_0^\infty rdr\Big\{(4m)^{-1}[(d\delta/dr)^2\\&+(r^{-1}q(r)\delta^2]+[-|\alpha'|(\delta^2-1)+\tfrac{1}{2}|\alpha'|(\delta^4-1)]\Big\}\\&+(8\pi)^{-1}\int H^2d^3x-(c/4e)H_aL,\end{aligned} \tag{23}$$

with

$$|\Psi_0|^2=7\zeta(3)N\Delta_\infty^2/8(\pi T_c)^2,$$

and

$$|\alpha'|=(1-T/T_c)6(\pi T_c)^2/7\zeta(3)E_F,$$

where

$$N=p_F^3/3\pi^2$$

is the electron density. Equation (23) was first derived by Gor'kov using a Green's-function technique.[4]

III. PERTURBATION THEORY

It is desirable to show that $\Delta G^{(1)}=0$ for arbitrary (analytic) variational potentials employed in calculating ΔG. For a vortex these potentials, $\delta(r)$ and $q(r)$, are large and what we have to say here cannot really apply. For in fact we show that if

$$\delta(x)=[1-\epsilon f(x,b)], \tag{24}$$

and

$$F(x)=\epsilon g(x,b), \tag{25}$$

that the term in $\Delta G^{(1)}$ linear in ϵ vanishes. It remains desirable to show that $\Delta G^{(1)}$ vanishes when $\epsilon\simeq1$.

The potentials of Eqs. (1) and (2) could possibly represent those of a magnetic impurity in a superconductor. To keep close ties with the vortex problem however, it will be assumed that the geometry of our problem is cylindrical. In particular we show that

$$\lambda_i(b)=E_i(b)/\Delta_\infty \simeq 1-\epsilon^2 z(b)\,,$$

and that to order ϵ, $\Sigma(\lambda,b)=C(b)/(\lambda^2-1)^{1/2}$.

We begin by considering the WKBJ equations for a bound state, suppressing the index b from f and g so that

$$\frac{d\omega}{dx}+[1-\epsilon f(x)]\cos\omega=\lambda+\epsilon g(x)\,. \tag{26}$$

Performing an expansion of ω in powers of ϵ

$$\omega=\omega^{(0)}+\omega^{(1)}+\cdots$$

and keeping only the first two terms one may show that

$$\omega^{(0)}=\cos^{-1}\lambda\,,$$

and that $\omega^{(1)}$ satisfies the equation

$$\frac{d\omega^{(1)}}{dx}-\omega^{(1)}(1-\lambda^2)^{1/2}=\epsilon(\lambda f(x)+g(x))\,. \tag{27}$$

This is a simple, linear, first-order differential equation with constant coefficients and is easily solved. The result is

$$\omega^{(1)}(x)=-\exp[(1-\lambda^2)^{1/2}x]\epsilon\int_x^\infty[\lambda f(x')+g(x')]\times\exp[-(1-\lambda^2)^{1/2}x']dx'\,, \tag{28}$$

and at $x=0$, we have

$$\omega(0)=\cos^{-1}\lambda-\epsilon\int_0^\infty[\lambda f(x)+g(x)]\times\exp[-(1-\lambda^2)^{1/2}x]dx+0(\epsilon^2)\,. \tag{29}$$

In order for the wave functions to be finite at the origin, $r=0$, $\omega(0)$ must vanish or be an integral multiple of π. The theory of a linear turning point in WKBJ theory brings this result about.

We expand $\lambda=1-\lambda^{(1)}$, and the eigenvalue equation is simply

$$\lambda^{(1)}=\tfrac{1}{2}\epsilon^2\left[\int_0^\infty[f(x)+g(x)]dx\right]^2 \tag{30}$$

to lowest order in ϵ so that there is no bound-state contribution to $\Delta G^{(1)}$ linear in ϵ.

For the scattering states, $\lambda\geq 1$, the function ω is in general complex:

$$\omega=\omega_1-i\omega_2\,.$$

Again performing an expansion of ω in powers of ϵ and keeping only terms linear in ϵ, we have

$$\omega_1^{(0)}=0\,,\quad \omega_2^{(0)}=\cosh^{-1}\lambda\,, \tag{31}$$

$$\omega^{(1)}=-\exp[-i(\lambda^2-1)^{1/2}x]\epsilon\int_x^\infty[\lambda f(x')+g(x')]\times\exp[i(\lambda^2-1)^{1/2}x']dx'\,, \tag{32}$$

and

$$\omega^{(1)}(0)=-\epsilon\int_0^\infty[\lambda f(x)+g(x)]\times\exp[i(\lambda^2-1)^{1/2}x]dx\,. \tag{33}$$

The expression for $\Sigma(\lambda,b)$ is given by Eqs. (15)–(17). To lowest order in ϵ the integral in $\sigma(b)$ is given by

$$I(b)=\int_0^\infty dx[\lambda\omega_2^{(1)}-\epsilon(\lambda^2-1)^{1/2}f(x)]\,, \tag{34}$$

and to lowest order in ϵ

$$\xi_1^+(0)+\xi_1^-(0)=\lambda\epsilon(\lambda^2-1)^{-1/2}\times\int_0^\infty[\lambda f(x)+g(x)]\cos[(\lambda^2-1)^{1/2}x]dx\,. \tag{35}$$

The integral $I(b)$ is equal to

$$I(b)=\int_0^\infty dx\bigg\{\lambda\epsilon\,\mathrm{Im}\exp[-i(\lambda^2-1)^{1/2}x]\times\int_x^\infty[\lambda f(x')+g(x')]\exp[i(\lambda^2-1)^{1/2}x']dx'-\epsilon(\lambda^2-1)^{1/2}f(x)\bigg\}\,. \tag{36}$$

Performing an integration by parts on the first term of Eq. (36) we have

$$I(b)=-\lambda\epsilon\bigg\{-(\lambda^2-1)^{-1/2}\int_0^\infty[\lambda f(x)+g(x)]dx+(\lambda^2-1)^{-1/2}\int_0^\infty[\lambda f(x)+g(x)]\times\cos[(\lambda^2-1)^{1/2}x]dx\bigg\}-\epsilon(\lambda^2-1)^{1/2}\int_0^\infty f(x)dx\,, \tag{37}$$

so that

$$\sigma(b)=\lambda\epsilon(\lambda^2-1)^{-1/2}\int_0^\infty g(x)dx+\epsilon(\lambda^2-1)^{-1/2}\int_0^\infty f(x)dx\,. \tag{38}$$

The function $g(x,b)$ is antisymmetric in b,

$$g(x,-b)=-g(x,b)\,, \tag{39}$$

and we have

$$\Sigma(\lambda,b)=\sigma(b)+\sigma(-b)=2\epsilon(\lambda^2-1)^{-1/2}\int_0^\infty f(x)dx. \quad (40)$$

Now the function $C(b)$ is given by

$$C(b)=\int_0^\infty [1-\delta^2(x)]dx=2\epsilon\int_0^\infty f(x)dx, \quad (41)$$

so that

$$\Sigma(\lambda,b)-C(b)(1-\lambda^2)^{-1/2}=0. \quad (42)$$

It does not seem possible to perform a Taylor expansion of $\Delta G^{(1)}$ in powers of ϵ beyond the linear term. It would seem necessary to adopt some other procedure to show that $\Delta G^{(1)}=0$ for $\epsilon\simeq 1$.

A numerical demonstration of $\Delta G^{(1)}=0$ has been made for the variational functions given in the Introduction.[5]

IV. GINZBURG-LANDAU FREE ENERGY

In the GL region, $T\simeq T_c$, the free-energy difference between a superconductor containing one vortex and a superconductor in the Meissner state, is given by Eq. (23). The variational potentials employed by Bardeen *et al.* are listed in the Introduction. The expression for the free-energy difference can be simplified to

$$\frac{\Delta G_s}{(L\pi\xi^2)N(0)\Delta_\infty^2}=\left(1-\frac{T}{T_c}\right)\left\{\int_0^\infty dr\left[\tfrac{1}{3}\pi^2 r\,\mathrm{sech}^4 r + \tfrac{1}{3}\pi^2\,\mathrm{sech}^2\left(\frac{sr}{d}\right)\frac{\tanh^2 r}{r} + r\,\mathrm{sech}^4 r\left(\frac{s}{d}\right)^2\frac{1}{s^2}\right] + 0.77\kappa^2 s^2 - 2\sqrt{2}\kappa\frac{H_{c1}}{H_c}\right\}. \quad (43)$$

The free energy is minimized with respect to s and s/d:

$$\frac{d\Delta F}{ds/d}=0, \quad \frac{d\Delta F}{ds}=0.$$

The GL parameter κ is solved for in terms of s and s in terms of s/d. H_{c1}/H_c can then be solved for in terms of κ by letting $\Delta G_s=0$. A plot of H_{c1}/H_c versus κ is shown in Fig. 1.

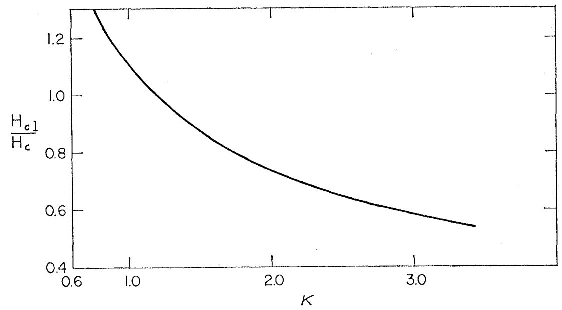

FIG. 1. Plot of H_{c1} versus κ for a clean type-II superconductor near T_c. The variational functions of Bardeen *et al.* have been employed in the calculation. The critical value of κ is found when $H_{c1}=H_c$. We find $\kappa_c=1.165$. This corresponds to a Ginzburg-Landau value of κ_c near $1/\sqrt{2}$.

The critical value of κ is found to be $\kappa_c(T_c)=1.165$, with the defining equation

$$\kappa(T)=c/2\sqrt{2}eH_c(T)\xi(T)^2. \quad (44)$$

Note that if we take the usual definition of $\kappa_{GL}(T_c)$, first introduced by GL and defined with

$$\lim_{T\to T_c}\xi_{GL}(T)=\frac{\pi}{4\gamma}(7\zeta(3)/3)^{1/2}\xi_0[T_c/(T_c-T)]^{1/2} \simeq 0.739\xi_0[T_c/(T_c-T)]^{1/2}, \quad (45)$$

where $\ln\gamma$ is Euler's constant, instead of using the parameter

$$\lim_{T\to T_c}\xi(T)=\frac{1}{\gamma}(7\zeta(3)/8)^{1/2}\xi_0[T_c/(T_c-T)]^{1/2} \simeq 0.576\xi_0[T_c/(T_c-T)]^{1/2}, \quad (46)$$

we have

$$\kappa_{GL}(T_c)/\kappa(T_c)=6/\pi^2, \quad (47)$$

so that $\kappa_{GLc}(T_c)=0.7082\simeq 1/\sqrt{2}$. This would indicate that the variational calculation is a good one, at least near T_c.

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