One virtue of these results is that they give confidence in the prescription of β from spectroscopic data as an effective pseudopotential for the transition metals. This is extremely valuable since pseudopotential calculations for these materials have not been done. The technique is, in principle, extendable to compounds and perhaps even alloys. The simplest approximation would be to take as a pseudopotential the sum of the "atomic" potentials of every atom in the unit cell along with the appropriate structure factors. An extension of this type would allow a great simplification in the calculation of many properties for these materials.

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[4]W. A. Harrison, *Pseudopotential in the Theory of Metals* (Benjamin, New York, 1966).

[5]The "best" values of Fig. 1 are taken from A. O. E. Animalu and V. Heine, Phil. Mag. 12, 1249 (1965) (tabulated values given in Ref. 4); A. O. E. Animalu, Proc. Roy. Soc. (London) 294, 376 (1966); J. A. Moriarty, Phys. Rev. B 1, 1363 (1970), where β is evaluated at $q = 2k_F$. The range of values given come both from other sources (see Ref. 4 and Allen and Cohen, Ref. 2) and the evaluation of β at the point where the pseudopotential equals zero. The ranges given then denote a range of "reliability" for the point-ion pseudopotential approximation for the metal.

[6]C. E. Moore, *Atomic Energy Levels*, NBS circular No. 467 (U. S. GPO, Washington, D. C., 1949, 1952, 1958), Vols. I–III.

[7]One could, of course, fit the data of Fig. 1 in a number of ways (e. g., a straight line with a positive intercept at $E_1 V_{at} = 0$). Alternative choices cause no qualitative changes in the results presented here, the only effect being a shift in the values of Δ [Eqs. (5) and (6)]. Lacking a real theoretical model for Eq. (3) or its equivalent, it does not pay to get any fancier. Equation (3) has the simple result that for the transition metals $\beta \simeq E_1 V_{at}$.

[8]K. A. Gschneidner, Jr., in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic, New York, 1964), Vol. 16.

[9]The one great deviation is for Ag, and results from the fact that E_1 in this case is quite large, of the order found for typical nontransition metals. The values of E_1 found for the related elements Cu and Au are much smaller. Why this difference occurs is not understood.

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Healing Length of the Superconducting Order Parameter*

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Using the Bardeen-Kümmel-Jacobs-Tewordt approach to the BCS theory of a nonuniform superconductor, we study the problem of a semi-infinite superconductor with a rigid potential barrier at the interface. Very close to T_c, the spatial variation of the order parameter is given by the Ginzburg-Landau formula $\Delta(z, T)/\Delta_\infty(T) = \tanh[z/\sqrt{2}\,\xi_{GL}(T)]$. At decreasing temperatures, however, the order parameter heals much more rapidly than $\xi(T) = v_F/\pi\Delta_\infty(T)$, where $\xi_{GL}(T) = \lim 0.74\,\xi(T)$ as $T \to T_c$; and, at low and intermediate temperatures, does so over atomic distances.

I. INTRODUCTION

Very close to T_c, if the superconducting order parameter is required to vanish on a plane, it heals as the hyperbolic tangent, $\Delta(z, T) = \Delta_\infty(T) \times \tanh[z/\sqrt{2}\xi_{GL}(T)]$, in an approximate length $\sqrt{2}\xi_{GL}(T)$.[1] Here $\xi_{GL}(T)$ is the coherence length of Ginzburg-Landau.[2] The technique of Bardeen, Kümmel, Jacobs, and Tewordt (BKJT) for calculating vortex structure lends itself well to a variational calculation of the healing length below the immediate vicinity of T_c.[3] Only modification of the

equations to reflect the new geometry is required.

In the vortex problem, the pair-breaking properties of the magnetic flux depress the order parameter from its uniform value at infinity to zero along the vortex axis. Self-consistency is maintained along the axis where all the electronic wave functions vanish. In the plane-boundary problem studied, the wave functions are forced to vanish identically on the plane and no magnetic field is introduced in the superconducting region. With this boundary condition, the free-energy difference is calculated between a superconductor with a finite healing length and that of a uniform superconductor. A minimum in the free energy, with a variational function for the order parameter, is arrived at by varying a parameter in the trial function. An optimized value for the healing length is thus obtained. It is also verified that the superconductor with a finite healing length has lower free energy.

In Sec. II some of the salient features of the BKJT theory are reviewed, and in Sec. III comment is made on our numerical techniques and results.

II. BKJT FORMALISM

The Bogoliubov equations for the wave functions of superconducting electronic excitations are

$$[E-(\tau^{(3)}/2m)(-\nabla^2-p_F^2)-\Delta(z)\tau^{(1)}]\times\Psi_E(x,y,z)=0, \tag{1}$$

where E is the energy, $\Delta(z)$ is the superconducting order parameter, and we have employed matrix notation.[4] The medium is translationally invariant in the x and y directions and the wave function is required to vanish at $z=0$, so that we have

$$\Psi_E=\Phi_{\vec{q},k}(z)\,e^{i\vec{q}\cdot\vec{\rho}}, \tag{2}$$

where $\vec{\rho}=(x,y)$

and

$$\Phi_{\vec{q},k}(0)=0. \tag{3}$$

Assuming that $\Delta(z)$ varies slowly over the length scale p_F^{-1}, a WKBJ approximation is made,[5]

$$\Phi_{\vec{q},k}(z)=g(z)\,e^{i(kz+\pi/2)}+\text{c.c.} \tag{4}$$

Equation (4) is substituted in (2) and (2) into (1), and second-order derivatives of g are neglected. The simplified equation is given by

$$-2i\tau^{(3)}\frac{dg}{d\zeta}=\lambda g-\frac{\Delta(\zeta)}{\Delta_\infty}\tau^{(1)}g, \tag{5}$$

where

$$\lambda=E/\Delta_\infty(T) \tag{6}$$

and

$$\zeta=(2m\Delta_\infty/k)z\,. \tag{7}$$

The subsidiary condition

$$q^2+k^2=p_F^2 \tag{8}$$

must be satisfied so that one may write

$$k=p_f\sin\alpha. \tag{9}$$

To simplify the numerical analysis, BKJT have written[3]

$$g=\begin{pmatrix}e^{i\eta/2}\\ e^{-i\eta/2}\end{pmatrix}e^{i\xi}, \tag{10}$$

and the equations satisfied by η and ξ are

$$\frac{d\eta}{d\xi}+\frac{\Delta(\zeta)}{\Delta_\infty(T)}\cos\eta=\lambda \tag{11}$$

and

$$2\frac{d\xi}{d\zeta}=i\frac{\Delta(\zeta)}{\Delta_\infty(T)}\sin\eta\,. \tag{12}$$

For bound states, $\lambda<1$, η is real, and ξ pure imaginary. The boundary condition imposed becomes, for $\eta(0)$,

$$\eta(0)=0,\ \pm2\pi,\ \pm4\pi,\ \text{etc.},$$

and one may see that

$$\eta(0)=\pm\pi,\ \pm3\pi,\ \pm5\pi,\ \text{etc.},$$

also produces valid bound states.

For $\lambda>1$, there is a continuum of scattering states, each one of which is characterized by a phase shift given by

$$\sigma^{\pm}=\xi_1^{\pm}(0)+\tfrac{1}{2}\int_0^\infty\{[\Delta(\zeta)/\Delta_\infty]\times\cos\eta_1\sinh\eta_2 - (\lambda^2-1)^{1/2}\}\,d\zeta\,. \tag{13}$$

The functions η and ξ are, in this case, complex, the subscripts 1 and 2 denoting their real and negative imaginary parts. Also

$$\xi_1^{\pm}(0)=-\tan^{-1}\{\tan[\tfrac{1}{2}\eta_1(0)]\times\tanh[\tfrac{1}{2}\eta_2(0)]^{\pm1}\}. \tag{14}$$

The pair potential $\Delta(z)$ is obtained by minimizing the free-energy difference between a superconductor with the potential $\Delta(z)$ and that with $\Delta_\infty(T)\,\theta(z)$.[3,6] To simplify matters we introduce a single variational parameter a,

$$\delta(z)=\Delta(z)/\Delta_\infty=\tanh(az/\xi)=\tanh(b\zeta), \tag{15}$$

where

$$\xi(T)=v_F/\pi\Delta_\infty(T)\ \text{and}\ b=\tfrac{1}{2}\pi a\sin\alpha,$$

optimizing $a(T)$ by finding a minimum of[3]

$$\Delta G=\frac{Ap_F^2T_c}{\pi}\,\frac{T}{T_c}\left[\frac{-1}{c^2}\sum_i\int_0^c b\,db\,\ln\left(\frac{\cosh(\lambda_i(b)\,\Delta_\infty(T)/2T)}{\cosh(\Delta_\infty(T)/2T)}\right)+\frac{1}{2\pi c^2}\,\frac{\Delta_\infty(T)}{2T}\right.$$
$$\left.\times\int_0^c b\,db\int_1^\infty d\lambda\left(\Sigma(\lambda,b)-\frac{1}{2b(\lambda^2-1)^{1/2}}\right)\tanh\left(\frac{\lambda\Delta_\infty(T)}{2T}\right)\right], \tag{16}$$

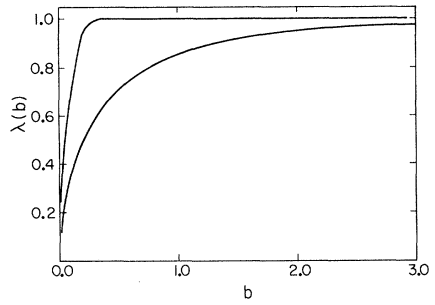

FIG. 1. Lowest two branches of bound-state spectrum. $b=\pi/2\sin\alpha$ a.

where

$$\Sigma=\sigma^{+}+\sigma^{-} \tag{17}$$

and

$$c=\tfrac{1}{2}\pi a\ .$$

$\lambda_i(b)$ is the ith branch of the bound-state spectrum. A is the area of the interface.

Near T_c, Eq. (16) becomes

$$\lim_{T\to T_c}\Delta G^{(1)}+\Delta G_{\mathrm{GL}},$$

where

$$\Delta G^{(1)}=\frac{Ap_F^2\,\Delta_\infty^2(T)}{4c^2\pi 2T}\int_0^c db\,\{\textstyle\sum_i b\tfrac{1}{2}\pi[1-\lambda_i^2(b)] + \int_1^\infty \lambda\,d\lambda\,[b\textstyle\sum(b,\lambda)-\tfrac{1}{2}(\lambda^2-1)^{-1/2}]\} \tag{18}$$

and ΔG_{GL} is the Ginzburg-Landau free energy as first derived from BCS theory by Gor'kov.[7,8] ΔG_{GL} is of order $\Delta_\infty^3(T)$ and presumably $\Delta G^{(1)}$ vanishes. Except for lowest-order perturbation theory, the only evidence for vanishing of $\Delta G^{(1)}$ is of a numerical nature and as such cannot be conclusive.[8,9] Assuming that $\Delta G^{(1)}$ does indeed vanish, we have $c(T_c)\simeq 0.869$.

III. NUMERICAL CALCULATIONS AND RESULTS

In Fig. 1 we plot $\lambda(b)$ for the two lowest branches of the bound-state spectrum. Using a technique by Bergk, one can see that for very small b the bound-state spectrum is given by

TABLE I. Numerical results for $c(T)$.

T/T_c	$c(T)$	$c(T)/c(T_c)$
1.0	0.869	1.0
0.98	1.05	1.21
0.96	1.20	1.38
0.94	1.40	1.61
0.92	1.90	2.21
0.90	>3.05	>3.51

$$\int_0^{\tanh^{-1}\lambda}\left(\frac{\lambda-\tanh x}{\lambda+\tanh x}\right)^{1/2}dx=b(i+\tfrac{1}{2})\tfrac{1}{2}\pi \tag{19}$$

except for λ very close to 1.[10] It follows that $d\lambda/db(\lambda=0)\to\infty$ for all i, so that the density of states for these branches is zero at the Fermi surface. For the vortex case, $(i+\frac{1}{2})$ in Eq. (19) is replaced simply by i because of the magnetic field, and there is one branch with $i=0$ which has a finite density of states at the Fermi surface. This is the branch which contributes to joule losses in flux flow.[11] Also, for small b

$$\textstyle\sum(b,\lambda)=b^{-1}\int_0^\infty[(\lambda^2-\tanh^2x)^{1/2}-(\lambda^2-1)^{1/2}]dx\ . \tag{20}$$

This formula was first derived for large λ by Bergk and Tewordt, but is applicable to almost all λ in our case, if b is sufficiently small.

Using the IBM system 360/75 at the University of Illinois Digital Computer Laboratory, numerical calculations of

$$\delta\Delta G/\delta c=0$$

were made for c values up to 3.05. Our results are tabulated in Table I. For $T=0.9T_c$, $c(0.9T_c)/c(T_c)>3.51$. Linearly extrapolating the data between T_c and $0.92T_c$, we have $c(0)\simeq 113$. Since this curve lies well below $c(0.90T_c)$, it can only be considered as a lower bound. It follows that at low and intermediate temperatures $c(T)\xi(T)\sim p_F^{-1}$, that is, the healing is over atomic distances.

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