Temperature and Purity Dependence of the Superconducting Critical Field H_{c2}. IV. Strong-Coupling Effects

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The existing theory of the transition temperature of a strong-phonon-coupling superconductor in zero magnetic field is merged with that of the upper critical field H_{c2} of a weak-coupling type-II superconductor to arrive at formulas for the strong-coupling corrections to $H_{c2}(T)$. A numerical computation is carried out for a phonon model of pure niobium. The strong-coupling effects make up only a negligible portion of the discrepancy between the earlier weak-coupling theory of H_{c2} and experimental observation, the remainder of which must be ascribed to Fermi-surface anisotropy.

I. INTRODUCTION

In previous articles,[1] an exact solution to the linearized Gor'kov equations in a uniform static magnetic field has been presented, yielding the second-order critical field H_{c2} of a bulk type-II superconductor. The solution covers the full temperature range and incorporates the effects of spin paramagnetism and impurity scattering.

Agreement of the calculated $H_{c2}(T)$ with experimental measurements has been good for superconducting alloys at low fields and satisfactory for high-field alloys where spin paramagnetism and spin-orbit impurity scattering become significant.[2] However, quantitative discrepancies exist with careful measurements on high-purity niobium[3] and vanadium,[4] which are intrinsically type-II superconductors. At low reduced temperatures, the measured values of H_{c2} for both of these materials lie about 15% above the theoretical prediction[1] for a pure sample.

Among the possible sources for the discrepancy, two are most likely: crystal structure, producing an anisotropy of the Fermi surface, and strong electron-phonon coupling effects. Both of these are omitted from the Gor'kov equations, which assume the simple BCS model potential and an isotropic material. The role of Fermi-surface anisotropy has recently been investigated by Hohenberg and Werthamer,[5] who found that it moved the theoretical H_{c2} curves in the direction of better agreement with the observations on Nb and V, although it was not possible to make quantitative calculations. In the present paper we correct the other deficiency in the earlier model, by calculating $H_{c2}(T)$ within the strong-phonon-coupling theory of superconductivity initiated by Eliashberg[6] and developed by Schrieffer, Scalapino, and Wilkins.[7]

In Sec. II we outline the merger of the existing theories of the transition temperature of a strong-coupling superconductor in zero field[6] with that of $H_{c2}(T)$ for a weak-coupling superconductor,[1] and arrive at formulas for the strong-coupling corrections to $H_{c2}(T)$. Since we allow for an arbitrary impurity concentration, these formulas are applicable to, and particularly relevant for, materials such as lead-based alloys. In Sec. III are presented results of a numerical computation of H_{c2} for a phonon model of pure Nb. It is found that the phonon effects make only a negligible contribution to the difference between the weak-coupling theory[1] and observation. Thus the discrepancy can presumably be ascribed entirely to Fermi-surface anisotropy.[5]

II. FORMAL SOLUTION

Following closely the development of Ref. 6 we begin by introducing the 2×2 Nambu[8] matrix single-particle Green's function $\mathcal{G}(x, x')$, where $x=(\mathbf{r}, t)$, appropriate for a coordinate-space description of the superconductor in a magnetic field. The Green's function satisfies Dyson's equation,

$$\mathcal{G}(x, x') = \mathcal{G}_n(x, x') + \int d^4x_1 d^4x_2 \mathcal{G}_n(x, x_1)\Sigma(x_1, x_2)\mathcal{G}(x_2, x'), \quad (1)$$

where $\mathcal{G}_n$ is the normal-state Green's function, containing the $\mathcal{G}_n$ magnetic field. The strong-coupling theory of superconductivity assumes the simple form

[1] E. Helfand and N. R. Werthamer, Phys. Rev. Letters **13**, 686 (1964); Phys. Rev. **147**, 288 (1966); N. R. Werthamer, E. Helfand, and P. C. Hohenberg, *ibid.* **147**, 295 (1966).

[2] R. R. Hake, Phys. Rev. Letters **15**, 865 (1965); Y. Shapira and L. J. Neuringer, Phys. Rev. **140**, A1638 (1965); L. J. Neuringer and Y. Shapira, Phys. Rev. Letters **17**, 81 (1966); J. A. Cape, Phys. Rev. **148**, 257 (1966).

[3] T. McConville and B. Serin, Phys. Rev. **140**, A1169 (1965); D. K. Finnemore, T. F. Stromberg, and C. A. Swenson, *ibid.* **149**, 231 (1966).

[4] R. Radebaugh and P. H. Keesom, Phys. Rev. **149**, 217 (1966).

[5] P. C. Hohenberg and N. R. Werthamer, Phys. Rev. **153**, 493 (1967).

[6] G. M. Eliashberg, Zh. Eksperim. i Teor. Fiz. **38**, 966 (1960) [English transl.: Soviet Phys.—JETP **11**, 696 (1960)].

[7] J. R. Schrieffer, D. J. Scalapino, and J. M. Wilkins, Phys. Rev. Letters **10**, 526 (1963); D. J. Scalapino, J. R. Schrieffer, and J. M. Wilkins, Phys. Rev. **148**, 263 (1966).

[8] Y. Nambu, Phys. Rev. **117**, 698 (1960).

for the matrix self-energy (vertex corrections can be shown to be negligible)

$$\Sigma(x, x') = -\tau_3 \mathcal{G}(x, x')[D(x, x') + nu^2\delta^3(\mathbf{r}-\mathbf{r}')]\tau_3, \quad (2)$$

where τ_3 is the third Pauli matrix in the 2×2 Nambu space, D is the phonon propagator, and nu^2 is the impurity concentration times the square of the impurity scattering amplitude. If we write the matrix Green's functions in the general form

$$\mathcal{G}_n(x, x') = \begin{pmatrix} G_n(x, x') & 0 \\ 0 & G_n(x', x) \end{pmatrix}, \quad (3a)$$

$$\mathcal{G}(x, x') = \begin{pmatrix} G_d(x, x') & G_{od}(x, x') \\ G_{od}^+(x, x') & G_d(x', x) \end{pmatrix}, \quad (3b)$$

then Eq. (1) can be split into two 1×1 equations for G_d and G_{od}. Since we are interested only in the second-order transition point, we can regard the off-diagonal (od) elements as infinitesimal. Linearizing the equations for G_d and G_{od} with respect to od elements, we arrive at

$$G_d(x, x') = G_n(x, x') + \int d^4x_1 d^4x_2\, G_n(x, x_1)\Sigma_d(x_1, x_2)G_d(x_2, x'), \quad (4)$$

$$G_{od}(x, x') = \int d^4x_1 d^4x_2\, G_n(x, x_1) \times[\Sigma_d(x_1, x_2)G_{od}(x_2, x') + \Sigma_{od}(x_1, x_2)G_d(x', x_2)], \quad (5)$$

or using Eq. (4) in (5),

$$G_{od}(x, x') = \int d^4x_1 d^4x_2\, G_d(x, x_1)\Sigma_{od}(x_1, x_2)G_d(x', x_2). \quad (6)$$

Neglecting anisotropy of the electron-band structure and of the phonon spectrum, it is appropriate[6] to assume that the phonon propagator has very short spatial range:

$$D(x, x') \cong D(t-t')\,\delta^3(\mathbf{r}-\mathbf{r}'). \quad (7)$$

Then using this together with Eq. (6) in Eq. (2), we find the linear homogeneous equation for Σ_{od}:

$$\Sigma_{od}(\mathbf{r}, \mathbf{r}; t-t') = [D(t-t') + nu^2]\int d^3r_1 dt_1 dt_2 \times G_d(\mathbf{r}, \mathbf{r}_1; t-t_1)\Sigma_{od}(\mathbf{r}_1, \mathbf{r}_1; t_1-t_2)G_d(\mathbf{r}, \mathbf{r}_1; t'-t_2). \quad (8)$$

The magnetic field appears[1] in the unperturbed Green's function, in the semiclassical approximation, as a phase factor:

$$G_n(x, x') = G_n(\mathbf{r}-\mathbf{r}'; t-t')\,\exp[i\varphi(\mathbf{r}, \mathbf{r}')], \quad (9)$$

$$\varphi(\mathbf{r}, \mathbf{r}') = (e/\hbar c)\int_{\mathbf{r}}^{\mathbf{r}'} d\mathbf{s}\cdot\mathbf{A}(\mathbf{s}), \quad (10)$$

where $\mathbf{A}$ is the vector potential and the integration follows a straight-line path between the end points. The phase integral form holds unchanged for G_d in the presence of the phonon interactions, because of approximation (7). This, together with Eq. (8), suggests that the space and time dependences of $\Sigma_{od}(\mathbf{r}, \mathbf{r}; t-t')$ factor:

$$\Sigma_{od}(\mathbf{r}, \mathbf{r}; t-t') = \Delta(\mathbf{r})\int d(\omega/2\pi)\,\exp[-i\omega(t-t')]\Phi(\omega). \quad (11)$$

The Ansatz (11) leads to the equation

$$\Delta(\mathbf{r})\Phi(\omega) = \int d(\omega_1/2\pi)[D(\omega-\omega_1) + 2\pi nu^2\delta(\omega-\omega_1)]\int d^3r_1 \times G_d(|\,\mathbf{r}-\mathbf{r}_1\,|; \omega_1)G_d(|\,\mathbf{r}-\mathbf{r}_1\,|; -\omega_1)\,\exp[2i\varphi(\mathbf{r}, \mathbf{r}_1)]\Delta(\mathbf{r}_1)\Phi(\omega_1). \quad (12)$$

The spatial part of Eq. (12) is now identical to the linear homogeneous integral equation solved in Ref. 1. Taking over the analysis of these references intact, we are led directly to the equation for $\Phi(\omega)$:

$$\Phi(\omega) = [1-nu^2 s(\omega)]^{-1}\int d(\omega_1/2\pi)\,D(\omega-\omega_1)s(\omega_1)\Phi(\omega_1), \quad (13)$$

where

$$s(\omega) = \int d^3r d^3r_1 \Delta(\mathbf{r})G_d(|\,\mathbf{r}-\mathbf{r}_1\,|; \omega)G_d(|\,\mathbf{r}-\mathbf{r}_1\,|; -\omega)\,\exp[2i\varphi(\mathbf{r}, \mathbf{r}_1)]\Delta(\mathbf{r}_1)/\int d^3r\,\Delta^2(\mathbf{r})$$

$$= \int d^3\rho G_d(\rho; \omega)G_d(\rho; -\omega)\,\exp(-eH\rho_\perp^2/2\hbar c), \quad (14)$$

and where $\rho_\perp$ is the magnitude of the projection of $\boldsymbol{\varrho}$ onto the plane perpendicular to the field **H**. We next introduce the form[1,6] for the normal-state Green's function,

$$G_d(\rho;\omega)=\int\frac{d^3p}{(2\pi)^3}\frac{\exp(i\mathbf{p}\cdot\boldsymbol{\varrho})}{Z(\omega)\omega-\epsilon(\mathbf{p})+i(\mathrm{sgn}\omega/2\tau)}, \quad (15)$$

which solves Eq. (4). Here $\epsilon(\mathbf{p})$ is the electron energy spectrum, $Z(\omega)$ is the phonon renormalization factor to be specified shortly, and τ is the impurity scattering time given by $(2\tau)^{-1}=2\pi N(0)nu^2$. Substituting Eq. (15) into Eq. (14), the ρ integration can be carried out[1] to yield

$$s(\omega)=\frac{2\pi iN(0)}{2Z(\omega)\,|\,\omega\,|+(i/\tau)}\int_0^\infty dw\,\exp(-w^2)\times\frac{1}{\alpha(\omega)}\ln\frac{1+\alpha(\omega)w}{1-\alpha(\omega)w}, \quad (16)$$

where

$$\alpha(\omega)=(2eH/\hbar c)^{1/2}v_F[2Z(\omega)\,|\,\omega\,|+(i/\tau)]^{-1}. \quad (17)$$

Also introducing an explicit expression for the phonon propagator in the manner of Ref. 6, we can fold the ω_1 contour to obtain

$$\tilde{\Phi}(\omega)\equiv\Phi(\omega)[1-nu^2s(\omega)]=\int_0^\infty d\omega_1\,K_+(\omega,\omega_1)\,\mathrm{Re}\left\{\tilde{\Phi}(\omega_1)\left[[Z(\omega_1)\omega_1+(2\tau)^{-1}]\left(\int_0^\infty dw\,\exp(-w^2)\frac{1}{\alpha(\omega_1)}\ln\frac{1+\alpha(\omega_1)w}{1-\alpha(\omega_1)w}\right)^{-1}-\frac{i}{2\tau}\right]^{-1}\right\}, \quad (18)$$

together with the relation for the renormalization factor,

$$\omega Z(\omega)=\omega-\int_0^\infty d\omega_1 K_-(\omega,\omega_1). \quad (19)$$

The kernels $K_\pm$ are given[6] by

$$K_\pm(\omega,\omega_1)=\sum_\lambda\int d\omega_\lambda F_\lambda(\omega_\lambda)\{(N(\omega_\lambda)+f(-\omega_1))((\omega_1+\omega_\lambda+\omega)^{-1}\pm(\omega_1+\omega_\lambda-\omega)^{-1})\mp(N(\omega_\lambda)+f(\omega_1))\times((-\omega_1+\omega_\lambda+\omega)^{-1}\pm(-\omega_1+\omega_\lambda-\omega)^{-1})\}, \quad (20)$$

where $F_\lambda(\omega_\lambda)$ is the coupling strength times density of states for phonons of frequency ω_λ in branch λ, and (N,f) are (boson, fermion) thermal weight factors. Equation (18) together with Eqs. (17), (19), and (20) constitute our final formal result, an eigenvalue equation determining the critical magnetic field H_{c2} as a function of temperature.

III. NUMERICAL RESULTS AND COMPARISON WITH EXPERIMENT

A numerical calculation of $H_{c2}(T)$ using the equations developed above was carried out for the case of pure niobium. The phonon density of states was taken from the neutron-scattering data of Nakagawa and Woods,[9] and a Coulomb pseudopotential, as discussed in Ref. 7, was chosen equal to 0.15. The last free parameter, the phonon-coupling strength, was then adjusted to give the observed zero-field transition temperature.

The most convenient way to plot the T dependence of H_{c2} is in terms of the dimensionless quantity[1]

$$h(t)\equiv H_{c2}(t)/(-dH_{c2}(t)/dt)_{t=1},$$

where t is the reduced temperature. The result of the numerical calculation is that $h(t)$ in the phonon model agrees with that given by the earlier weak-coupling solution to within 2%, the accuracy of the present program. The main effect of having included the phonon interactions is to alter the electron effective mass (or equivalently the Fermi velocity) from the band-mass value because of the renormalization constant $Z\neq1$. This produces a substantial over-all increase in H_{c2} from that which would be obtained using the bare band Fermi velocity, but being relatively temperature-independent the shift cancels out of $h(t)$. Since phonon coupling has proved to be of little significance in determining the temperature dependence (although not the magnitude) of H_{c2} for pure Nb, it would appear that the discrepancy between theory and experiment for both Nb and V must be attributed entirely to anisotropy of the Fermi surface.

It would be of some interest to learn whether phonon effects make any contribution to $h(t)$ for materials more strongly coupled than niobium, for instance alloys of lead.

[9] Y. Nakagawa and A. D. B. Woods, Phys. Rev. Letters **11**, 271 (1963).