Microscopic Description of the Vortex State near the Upper Critical Field

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We solve the BCS-Gor'kov equations for a pure, isotropic type-II superconductor near the upper critical field. Corrections to the semiclassical results lower the value of the upper critical field and cause $H_{c2}(T)$ to vanish quadratically near T_c. This form leads to positive curvature in the critical field, which has been seen in a range of materials, and means that a type-II superconductor will convert to type I at a temperature close to T_c.

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In 1959, Gor'kov derived an expression for the upper critical field of type-II superconductors at low temperature using his Green's function description of superconductivity and a semiclassical phase approximation [1]. Subsequent extensions to higher temperature and to theories including the effects of spin and impurities are the basis of the semiclassical theory of the phase transition [2,3]. In this Letter, we show that solving the BCS-Gor'kov theory near H_{c2} directly, by generalizing pairing between plane waves to pairing between many electronic Landau levels, can lead to significant deviations from the semiclassical results.

The starting point is the Hamiltonian proposed by Gor'kov, based on an interaction between electrons which is short range and attractive in a narrow energy range around the Fermi energy:

$$H = \int d\mathbf{r}\, c^\dagger_{\mathbf{r}\,\sigma} H_0(\mathbf{r}) c_{\mathbf{r}\,\sigma} - \frac{1}{2} V_0 \Omega \int d\mathbf{r}\, c^\dagger_{\mathbf{r}\sigma} c^\dagger_{\mathbf{r}\sigma'} c_{\mathbf{r}\sigma} c_{\mathbf{r}\sigma'}\,, \qquad (1)$$

in a volume Ω, $[c_{\mathbf{r}}, c^\dagger_{\mathbf{r}'}] = \delta^3(\mathbf{r}-\mathbf{r}')$, and $H_0(\mathbf{r}) \equiv (1/2m)[i\nabla - (e/c)\mathbf{A}(\mathbf{r})]^2 - E_F$. $V_0 > 0$ for particles with energy $|E - E_F| < E_p$ and zero outside this range. The variational approach to this problem is defined by

$$H' = \int d\mathbf{r} \begin{bmatrix} c^\dagger_{\mathbf{r}\uparrow} & c_{\mathbf{r}\downarrow} \end{bmatrix} \begin{bmatrix} H_0(\mathbf{r}) & \phi(\mathbf{r}) \\ \phi^*(\mathbf{r}) & -H_0^*(\mathbf{r}) \end{bmatrix} \begin{bmatrix} c_{\mathbf{r}\uparrow} \\ c^\dagger_{\mathbf{r}\downarrow} \end{bmatrix}, \qquad (2)$$

$$\phi(\mathbf{r}) = -V_0 \Omega \langle c_{\mathbf{r}\uparrow} c_{\mathbf{r}\downarrow} \rangle\,. \qquad (3)$$

The equations for the eigenfunctions of the matrix appearing in (2) are the Bogoliubov–de Gennes equations [4]. The BCS theory [5] is recovered when $\mathbf{A} = 0$ and $\phi(\mathbf{r})$ is constant: a plane wave basis reduces the matrix to uncoupled 2×2 matrices mixing $c_{\mathbf{k}}$ and $c_{-\mathbf{k}}$, and the self-consistency equation (3) to the BCS gap equation.

Because the magnetic field is uniform near H_{c2}, Landau levels are a better basis than plane waves. If the ground state has the form of a periodic vortex lattice, degenerate states within a Landau level are combined into eigenstates which conserve momentum with respect to that lattice. The equation which determines the upper critical field was derived from the Gor'kov equations in Ref. [6]. An alternative formulation using this basis shows why the divergences found there ($H_{c2} \to \infty$ as $T \to 0$) do not occur and illustrates some further points. The basis is

$$[H', c^\dagger_{\lambda\mathbf{p}\sigma}] = E_{\lambda\mathbf{p}} c^\dagger_{\lambda\mathbf{p}\sigma}\,, \qquad (4)$$

$$c^\dagger_{\lambda\mathbf{p}\uparrow} = \sum_n (u^\lambda_{n\mathbf{p}} c^\dagger_{n\mathbf{p}\uparrow} + v^\lambda_{n\mathbf{p}} c_{n,-\mathbf{p},\downarrow})\,, \qquad (5)$$

$$c^\dagger_{n\mathbf{p}\sigma} = \int d\mathbf{r}\, \psi^*_{n\mathbf{p}}(\mathbf{r}) c^\dagger_{\mathbf{r}\sigma}\,, \qquad (6)$$

$$\psi_{n\mathbf{p}}(\mathbf{r}) = (\sqrt{\pi}/\Omega)^{1/2} e^{ik_z z} \sum_s e^{isq_y b} e^{i(q_x + s\pi/b)x} \times h_n[\sqrt{\pi}(y/b + s + q_x b/\pi)]\,, \qquad (7)$$

$$h_n(x) = (-1)^n (\sqrt{\pi}\, 2^n\, n!)^{-1/2} e^{x^2/2} \frac{d^n}{dx^n} e^{-x^2}. \qquad (8)$$

The $c^\dagger_{\lambda\mathbf{p}\sigma}$'s are the quasiparticle operators that diagonalize the Hamiltonian; $\mathbf{p} \equiv (k_z, \mathbf{q})$, where $\hbar k_z$ is the ordinary z momentum and $\mathbf{q} = (q_x, q_y)$ are wave vectors defined with respect to the vortex lattice; $c^\dagger_{n\mathbf{p}\sigma}$ creates an electron in the nth Landau level with the periodicity of a square vortex lattice of side $b = l_H\sqrt{\pi}$ [7]; $\psi_{n\mathbf{p}}(\mathbf{r})$ is this magnetic Bloch state in the gauge $\mathbf{A} = Hy\,\hat{\mathbf{x}}$; s runs over all integers; and the Hermite functions $h_n(x)$ are normalized harmonic oscillator eigenstates.

In the BCS case the order parameter is a constant. In the vortex state the order parameter can be expanded in terms of "vortex lattice Hermite functions,"

$$\lambda_k(u,v) = (2\pi)^{1/4} \sum_s e^{2\pi i s u} h_k[\sqrt{2\pi}(s + v)]\,, \qquad (9)$$

orthonormal on the unit cell $0 < u, v < 1$. The phase of these functions winds by 2π about each of a square lattice of points $(u,v) = (\frac{1}{2} + j, \frac{1}{2} + k)$. λ_0 is the Abrikosov form for the order parameter [8], and the higher k functions can be expressed in terms of its derivatives. What makes these functions useful is that the momentum and position dependence of the pair product separate:

$$\psi_{m\mathbf{p}}(\mathbf{r})\psi_{n,-\mathbf{p}}(\mathbf{r}) = \frac{1}{\sqrt{2}\,\Omega} \sum_k C^k_{mn} \lambda_k(\mathbf{r}/b) \lambda_{m+n-k}(\mathbf{q}b/\pi)\,, \qquad (10)$$

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where the combinatorial factors C^k_{mn} are [9]

$$C^k_{mn} = [2^{-(m+n)} m!\, n!\, k!\, (m+n-k)!]^{1/2} \times \sum_s \frac{(-1)^s}{(m+n-k-s)!\,(k+s-n)!\,(n-s)!\,s!}, \quad (11)$$

and this simplifies the gap equation and matrix elements.

The pairing amplitudes in the Landau level basis are the eigenvectors of a large matrix that generalizes the 2×2 matrix in the BCS theory:

$$\begin{bmatrix} E^0(k_z) & A(\mathbf{p}) \\ A^\dagger(\mathbf{p}) & -E^0(k_z) \end{bmatrix} \begin{bmatrix} u^\lambda_{\mathbf{p}} \\ v^\lambda_{\mathbf{p}} \end{bmatrix} = E_{\lambda \mathbf{p}} \begin{bmatrix} u^\lambda_{\mathbf{p}} \\ v^\lambda_{\mathbf{p}} \end{bmatrix}, \quad (12)$$

where the pairing matrix element is

$$\begin{aligned} A_{mn}(\mathbf{p}) &= \int d\mathbf{r}\, \phi(\mathbf{r}) \psi_{m\mathbf{p}}(\mathbf{r}) \psi_{n,-\mathbf{p}}(\mathbf{r}) \\ &= \hbar\omega_H \sum_{k=0}^{m+n} \phi_k C^k_{mn} \lambda_{m+n-k}(\mathbf{q}b/\pi), \end{aligned} \quad (13)$$

in terms of the order parameter components

$$\phi_k = \frac{1}{\sqrt{2}\,\Omega\,\hbar\omega_H} \int d\mathbf{r}\, \lambda_k(\mathbf{r}/b) \phi(\mathbf{r}). \quad (14)$$

The bare energies in Eq. (12) are Landau levels

$$\begin{aligned} E^0_{mn}(k_z) &= \delta_{m,n} E^0_n(k_z) \\ E^0_n(k_z) &= [(n + 1/2)\hbar\omega_H + \hbar^2 k_z^2/2m - E_F], \end{aligned} \quad (15)$$

with $\omega_H = eH/mc$ and the restriction

$$|E^0_m(k_z)| < E_p, \qquad |E^0_n(k_z)| < E_p, \quad (16)$$

pairing only those levels within a cutoff energy E_p of the energy available for motion perpendicular to the field.

Near the phase transition, when $\phi(\mathbf{r})$ is small, the matrix of expectation values,

$$F_{mn}(\mathbf{p}) = \langle c_{m\mathbf{p}\uparrow} c_{n,-\mathbf{p}\downarrow} \rangle = \sum_{\lambda, E_\lambda > 0} u^\lambda_{m\mathbf{p}} v^{\lambda *}_{n\mathbf{p}}, \quad (17)$$

can be calculated using perturbation theory

$$F_{mn}(\mathbf{p}) = -\frac{A_{mn}(\mathbf{p})}{|E^0_m + E^0_n|} \theta(E^0_m E^0_n) + O(\phi^3), \quad (18)$$

where $\theta(x) = 1$ for $x > 0$ and 0 for $x < 0$. Equations (6), (10), (13), and (18), together with the orthogonality of the λ_k's, yield for the self-consistency equation (3) one gap equation for each component ϕ_k:

$$\begin{aligned} \phi_k \neq 0 &\Leftrightarrow g > g_k(H) \\ &\Leftrightarrow H < H_k, \end{aligned} \quad (19)$$

where H_k is defined through

$$g_k(H_k) = g, \quad (20)$$

g is the BCS coupling constant,

$$g = V_0 \Omega m k_F / 2\pi^2 = V_0 N(E_F), \quad (21)$$

and the functions $g_k(H)$ are given by

$$\begin{aligned} g_k(H)^{-1} = \frac{1}{2} \int_0^{k_F} \frac{dk_z}{k_F} \sum_{m,n} \frac{(C^k_{mn})^2}{|E^0_m + E^0_n|} \hbar\omega_H \\ \times \theta(E^0_m E^0_n)\, \theta(E_p - |E^0_m|)\, \theta(E_p - |E^0_n|). \end{aligned} \quad (22)$$

The upper critical field for the vortex state is defined by the largest H_k, which occurs for $k = 0$.

The points $E^0_m = E^0_n = 0$ do not contribute to a divergence because the perturbative expansion (18) does not apply there. Diagonalizing these levels exactly shows that they lead to tails of persisting superconductivity just above H_{c2} whose effects vanish in the limit $E_F \gg \hbar\omega_H$ that applies to conventional superconductors.

In the limit of many paired N_p and filled N_f Landau levels,

$$N_p = \frac{E_p}{\hbar\omega_H}, \qquad N_f = \frac{E_F}{\hbar\omega_H}. \quad (23)$$

we can use the asymptotic form

$$(C^0_{N+s,N-s})^2 = e^{-s^2/N} / \sqrt{\pi N}, \quad (24)$$

and write the equation for H_{c2}, Eq. (20) with $k = 0$, as

$$\frac{1}{g} = \int_0^{k_F} \frac{dk_z}{k_F} \int_0^{\Gamma_z} \int_0^{\min(x, \Gamma_z - x)} dx\, dy\, \frac{2}{\sqrt{\pi}} \frac{e^{-y^2}}{x} \quad (25)$$

$$= \int_0^{k_F} \frac{dk_z}{k_F} [\ln(2\Gamma_z) + \mathbf{C}/2 + O(1/\Gamma_z)], \quad (26)$$

$$\Gamma_z \equiv N_p / \sqrt{N_f (1 - k_z^2/k_F^2)},$$

where $\mathbf{C}$ is the Euler constant ≈ 0.577, and we have assumed small E_p/E_F. Doing the k_z integral, we obtain $O(\sqrt{N_f}/N_p)$:

$$g^{-1} = \ln[a N_p / \sqrt{N_f}], \qquad a = e^{1 + \mathbf{C}/2}. \quad (27)$$

The BCS zero-field gap equation has a sum over $1/E$ similar to Eq. (22) which yields $1/g = \ln[2E_p/\Delta_0]$ for small Δ_0. This has a solution for arbitrarily weak coupling, the BCS instability. Using the definitions for N_p and N_f shows that in the vortex state this has been replaced by $\ln[\alpha E_p/\sqrt{H}]$, with $\alpha^2 = 2a^2 \Phi_0 / \pi \hbar^2 v_F^2$ and Φ_0 the flux quantum $hc/2e$. The magnetic field cuts off the BCS instability and creates a minimum coupling strength, Eq. (19), which defines the upper critical field.

Using the BCS weak-coupling values, $\Delta_0 = 2E_p \exp[-1/g]$ and $\xi_0 = \hbar v_F/\pi\Delta_0$, and the solution to Eq. (27) as $H = H_{c2}^0$ yields

$$H_{c2}^0 = \frac{a^2}{2\pi^3}\frac{\Phi_0}{\xi_0^2} = 0.212\,\frac{\Phi_0}{\xi_0^2}\,. \tag{28}$$

The semiclassical result is $H_{c2}^S = 1.26\sqrt{2}\,\kappa_0 H_c$ [1,2], where κ_0 is the Ginzburg-Landau parameter at T_c, $\kappa_0 = 0.958\lambda_L/\xi_0$, H_c is the thermodynamic critical field $2[\pi N(E_F)]^{1/2}\Delta_0$, and λ_L is the London penetration depth $[mc^2/4\pi\rho e^2]^{1/2}$. These yield $H_{c2}^S = 0.212(\Phi_0/\xi_0^2)$.

The quantum and semiclassical results for H_{c2} agree with $O(\sqrt{N_f/N_p})$, that correction coming from the $O(1/\Gamma_z)$ term in Eq. (26). It follows from (27) that the size of this correction is $O(e^{-1/g})$. This indicates a much greater sensitivity to the cutoff of the pairing potential than is usually present in BCS, where strong-coupling corrections derived from the Eliashberg equations are the square of this: $O(T_c/E_p)^2$. Doing the integrals numerically shows that, for typical values $g = 0.2$–0.4, $H_{c2}(0)$ is decreased relative to the value (28) by 2%–23%, as shown in Fig. 1.

To estimate the sensitivity of this effect to impurities, we broaden the bare energies by an amount $i\hbar/\tau$. Repeating the steps that led to Eq. (25) gives $\ln(H_{c2}/H_{c2}^0) = O(\sqrt{N_f/N_p}) + O((\omega_H\tau)^{-1}/\sqrt{N_f})$. The factor $1/\sqrt{N_f}$ in the second term shows that scattering becomes important not when $\omega_H\tau \sim 1$ but when the mean free path $v_F\tau \sim l_H$. This is the standard semiclassical criterion for the clean limit.

Experimental results are usually expressed in terms of the slope of $H_{c2}(T)$ at T_c. The temperature dependence of H_{c2} is given by replacing $\theta(E_m^0 E_n^0)/|E_m^0 + E_n^0|$ in Eq. (22) with $[\tanh(\beta E_m^0/2) + \tanh(\beta E_n^0/2)]/2(E_m^0 + E_n^0)$. This yields

$$\begin{aligned}\frac{1}{g} &= \int_0^{k_F}\frac{dk_z}{k_F}\int_0^{\beta E_p}\frac{du}{u}\int_0^{\beta E_p} dv \\ &\quad\times \frac{e^{-v^2/\epsilon_z^2}}{\sqrt{\pi}\,\epsilon_z}\,\frac{2\sinh u}{\cosh u + \cosh v}\,\theta(\beta E_p - u - v) \\ \epsilon_z^2 &\equiv \beta^2\,\hbar\omega_H E_F(1 - k_z^2/k_F^2)\,. \end{aligned}\tag{29}$$

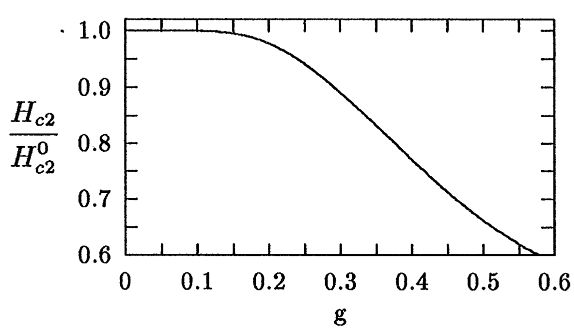

FIG. 1. $H_{c2}(T=0)$ relative to the semiclassical result as a function of BCS coupling constant.

When $H = 0$ this is the BCS equation for T_c. For any H, Eq. (29) can be expressed in terms of the dimensionless variables

$$h \equiv H/H_{c2}^0, \qquad t \equiv T/T_c$$

and constants which depend only on g. Expanding the integrals near T_c then yields, to first order in $e^{-1/g}$,

$$0 = 1.61e^{-1/g}\sqrt{h} + 0.727h - \delta t\,, \tag{30}$$

where $\delta t = 1 - t$. In the limit $g \to 0$, the semiclassical result $h^*(0) \equiv 1/(dh/dt)_{t=1} = -0.727$ is recovered. For $g \neq 0$, however, the presence of the $\sqrt{h}$ term causes $H_{c2}(T)$ to vanish quadratically near T_c, not linearly, as in the semiclassical theory. These results are illustrated in Fig. 2.

In practice, this means that near T_c the slope of the upper critical field decreases until H_{c2} falls below H_c, at which point the material becomes type I and the field being measured is the thermodynamical critical field. This would be manifested as a small upturn in the upper critical field near T_c. Such upturns were first seen weakly in older experiments on single-crystal vanadium [11], then more clearly on the A15 compounds [12,13]. The upturn is most evident for the cleaner Nb_3Sn samples and present, but significantly less, in the clean V_3Si sample of Ref. [13]. Since the degree to which the upturn is present depends on T_c/E_p, such a difference would be expected from the similar T_c's but lower Debye energy

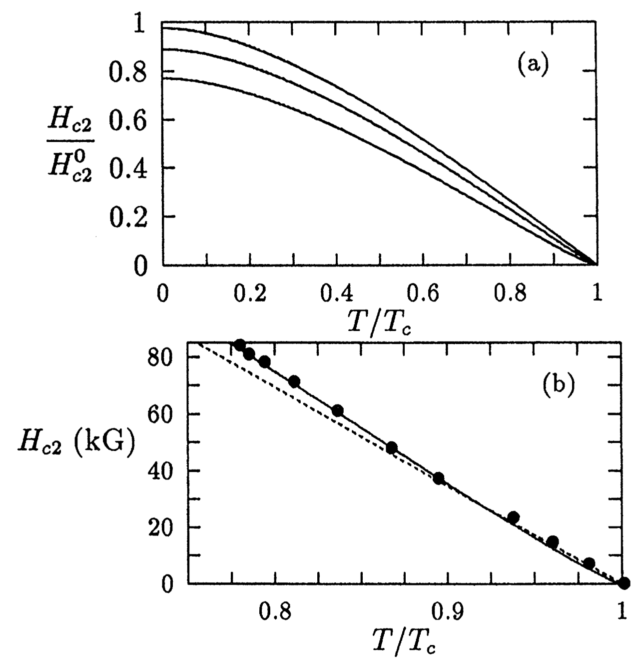

FIG. 2. $H_{c2}(T)$: (a) relative to the $T = 0$ semiclassical value for $g = 0.2, 0.3, 0.4$ (top, middle, lower lines), and (b) near T_c for $g = 0.3$, fit to $H_{c2}^0 = 320\,\text{kG}$. Points and dashed line are data and fit by semiclassical theory for Nb_3Sn from Ref. [13].

for Nb_3Sn. An upturn near T_c has also been seen in the Chevrel material Mo_6Se_8 [14].

Inhomogeneities have been offered as an explanation for such upturns. However, the curvature increases as the materials get cleaner, as measured by normal-state resistivity. Fermi surface anisotropy is also a problematic explanation: it seems to be too small to explain the upturns in the A15's [12,15]. The presence of a small intrinsic $\sqrt{h}$ term appears to be a more natural explanation. Measuring the inhomogeneity in H_{c2} across the material would be an important test in establishing this. The most direct test would be observing a transition from a type-II to a type-I superconductor, as might be seen by magnetization measurements or the presence of hysteresis.

Previous discussions of the upper critical field have focused on larger measured values of $h^*(0)$ than predicted by the semiclassical theory [11–17]. In the A15 compounds [13] and Chevrel materials [14,16], the critical fields can get large enough that Pauli paramagnetic limiting becomes important. In these cases an absence of such limiting was found (more pronounced in Nb_3Sn than V_3Si), which is difficult to explain within the context of the semiclassical theory [15]. A decreasing slope near T_c, however, raises $h^*(0)$. A model including the effects of Pauli limiting, impurity scattering, and a realistic phonon propagator as well as a better understanding of the resistive transition and more data near T_c will be important for a more quantitative comparison.

Experiments on heavy fermion superconductors also indicate a positive curvature near T_c [18], however, it is less likely that the conventional s-wave BCS-Gor'kov model applies to those materials or the high-T_c materials, where the effects of strong anisotropy may be important.

Away from H_{c2}, the density of states of the Hamiltonian [Eq. (12)] has a characteristic form. In the normal state, the spectrum is flat in the narrow energy range relevant for superconductivity. When the pairing is turned on, off-diagonal matrix elements cause the eigenvalues of this large matrix to repel, and the effect is to turn the flat density of states into a dimple around the Fermi energy. The depth of this dimple is related to the size of the matrix and the strength of the order parameter. In numerical simulations with parameters close to those of typical materials, we find that such a dimple develops and deepens gradually as the magnetic field decreases away from H_{c2}. This gapless form should hold down to H_{c1}. The presence of such excitations is indicated by the persistence of magnetic oscillations [19] and by scanning tunneling microscopy measurements at fields well below H_{c2} and positions midway between what are ordinarily considered vortex cores [20]. This suggests that it would be interesting to reexamine the fully self-consistent solution for an isolated vortex.

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