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Excitations in the mixed state of type-II superconductors

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Quasiparticle excitations in the mixed state of a type-II superconductor outside the vortex cores are shown to fall into bands, and near H_{c2} have a Landau-level type of structure. This leads to de Haas–van Alphen oscillations in the quasiparticle magnetization. Most of the pairing comes from states near the band edges and gives rise to a complicated structure of the order parameter.

There has been considerable interest recently in the spectrum of quasiparticle (qp) excitations in the mixed state of type-II superconductors. Scanning-tunneling-microscope techniques have been used to study the local density of states in the cores of the vortices.[1] The bound states, density of states, and scattering states of a single vortex line have been studied theoretically by a number of authors.[2–7] The bound states in the cores of the vortex lines are, to a first approximation, independent of the field when the coherence length is small. The effect of the periodic lattice of vortex lines on these states has been discussed by Canel.[8] If the temperature is not too low, most of the excitations—for materials with a small coherence length—will lie outside the cores; these excitations can make a contribution to the thermodynamic properties of the superconductor. In the present paper we study the quasiparticle excitations above the gap outside the vortex cores. They have an interesting structure and fall into bands and near H_{c2} have a Landau-level-type structure. This leads to de Haas–van Alphen-like oscillations in the quasiparticle magnetization. de Haas–van Alphen oscillations in the mixed state have been observed by Graebner and Robbins.[9]

From the quasiparticle spectrum the order parameter can be calculated self-consistently. Our results show that most of the pairing comes from states near the quasiparticle band edges. The order parameter also contains contributions from higher Landau levels and thus has a more complicated structure than that given by Abrikosov.[10] Such contributions have been discussed by Markiewicz *et al.*[11] but were based on some *ad hoc* assumptions about pairing in the mixed state. de Haas–van Alphen oscillations in the critical temperature in the high-magnetic-field limit have been studied by Gruenberg and Gunther[12] and Tesanovic, Rasolt, and Xing.[13]

The quasiparticle excitations in a superconductor are solutions to the Bogoliubov equations[14] for the amplitudes u and v

$$\left[\frac{1}{2m_e}(\mathbf{p}-e\mathbf{A}/c)^2-\varepsilon_F\right]u+\Delta(r)v=Eu\,,$$
$$-\left[\frac{1}{2m_e}(\mathbf{p}+e\mathbf{A}/c)^2-\varepsilon_F\right]v+\Delta^*(r)u=Ev\,, \tag{1}$$

where ε_F is the Fermi energy. We first study the excitations near H_{c2} and we take the order parameter in the Abrikosov form

$$\Delta(r)=\Delta\sum_n e^{iqny}\exp[-(x-nql^2)^2/2l^2]\,, \tag{2}$$

where $l^2=c/2eH_{c2}$ and

$$\Delta^2=\frac{6\pi^3T_c^2}{7\zeta(3)}\frac{m_eH_{c2}^2l^2K}{(2m_e\varepsilon_F)^{3/2}}\frac{(1-H/H_{c2})}{\beta(1-\frac{1}{2}K^2)}\,.$$

For simplicity we assume a square flux-line lattice with $q^2=2\pi/l^2$ but this has little effect on the results. The form (2) for Δ corresponds to a vector potential $\mathbf{A}=(0,Hx,0)$. K is the Ginzburg-Landau parameter. In (1) we take the vector potential as that of a uniform field, i.e., as above, and neglect its variation due to the vortices, which is of order Δ^2. The order parameter is periodic in y and we can write the solutions of (1) in the Bloch form

$$u=\sum_n e^{i(k+nq)y}u_n^{(k)}(x)\,,$$
$$v=\sum_n e^{i(k-nq)y}v_n^{(k)}(x)\,, \tag{3}$$

with $-q/2<k\le q/2$. For simplicity we consider the two-dimensional case. The modifications for three dimensions are given below. When (3) are substituted in (1) we get the set of equations

$$\frac{1}{2m}\left[-\frac{d^2}{dx^2}+\left(nq+k-\frac{x}{2l^2}\right)^2-k_F^2\right]u_n^{(k)}+\Delta\sum_{n'}f_{n'}v_{n'-n}^{(k)}=Eu_n^{(k)}\,,$$
$$-\frac{1}{2m}\left[-\frac{d^2}{dx^2}+\left(nq-k-\frac{x}{2l^2}\right)^2-k_F^2\right]v_n^{(k)}+\Delta\sum_{n'}f_{n'}u_{n'-n}^{(k)}=Ev_n^{(k)}\,, \quad (4)$$

where $f_n = e^{-(x-nql^2)^2/2l^2}$.

In the absence of pairing ($\Delta=0$) the solutions of (4) are normalized harmonic-oscillator functions $\psi_m\{[x-2l^2(nq\pm k)]/2l^2\}$ of width $\sqrt{2}l$ centered around $x=2l^2(nq\pm k)$, and of energy $\varepsilon_m=(m+\frac{1}{2})\omega_c-\varepsilon_F$ where $\omega_c=eH/m_e c$ is the cyclotron frequency. They are thus strongly localized as are the functions f_n. In obtaining approximate solutions to (4), as $\Delta\ll\omega_c$ we can neglect mixing of different Landau levels through Δ. If necessary this could be included by perturbation theory. Also as the functions in (4) are strongly localized a tight-binding approximation is suitable. From (4) we see that the strongest pairing will occur near the edges of the bands, i.e., for $k=0$ the pairing occurs between u_n and v_n which have the largest overlap, and for $k=q/2$ between u_n and v_{n+1}. We first examine these two cases.

(i) $k=0$. We only retain the amplitudes u_n and v_n in (4) which become

$$\frac{1}{2m}\left[-\frac{d^2}{dx^2}+\left(nq-\frac{x}{2l^2}\right)^2-k_F^2\right]u_n+\Delta f_{2n}v_n=Eu_n\,,$$
$$-\frac{1}{2m}\left[-\frac{d^2}{dx^2}+\left(nq-\frac{x}{2l^2}\right)^2-k_F^2\right]v_n+\Delta f_{2n}u_n=Ev_n\,. \quad (5)$$

As Δ is small the approximate solutions are

$$\begin{pmatrix}u_n\\v_n\end{pmatrix}=\begin{pmatrix}a_n\\b_n\end{pmatrix}\psi_m(x-2l^2nq)\equiv\begin{pmatrix}a_n\\b_n\end{pmatrix}\psi_m^{(n)}\,, \quad (6)$$

where ψ_m is the mth normalized harmonic oscillator function. It should be noted that f_{2n} is large where u_n and v_n are large. When (6) is substituted in (5) and we multiply on the left by $\psi_m^{(n)}$ and integrate we get the equations

$$\varepsilon_m a+\Delta I_m b=Ea\,,\qquad -\varepsilon_m b+\Delta I_m a=Eb\,, \quad (7)$$

where

$$I_m=\int dx f_{2n}(\psi_m^{(n)})^2=\frac{(2m)!}{2^{2m+(1/2)}(m!)^2}\,. \quad (8)$$

From (7) the qp energies and amplitudes are independent of n and given by

$$E_m=(\varepsilon_m^2+\Delta^2 I_m^2)^{1/2}\,,\quad a^2=\frac{1}{2}\left(1-\frac{\varepsilon_m}{E_m}\right)\,,$$
$$b^2=\frac{1}{2}\left(1+\frac{\varepsilon_m}{E_m}\right)\,. \quad (9)$$

The quasiparticles thus have a Landau-level structure. In three dimensions E_m is replaced by $\varepsilon_{m,k}=\varepsilon_m+k_z^2/2m_e$, where k_z is the wave vector parallel to the vortex lines. The energy-gap parameter ΔI_m depends on the quantum number m; in particular $I_0=2^{-1/2}$ and for large m, $I_m\sim 1/(2\pi m)^{1/2}$.

(ii) $k=q/2$. In this case the largest coupling occurs between u_n and v_{n+1} through the term f_{2n+1} in (4) and an identical set of qp energies to (9) is obtained.

For $k=0$ or $q/2$ we have highly degenerate sets of solutions (6) for each value of m corresponding to the different values of n. When the interaction between these states is taken into account these solutions form bands. As the states u_n and v_n are strongly localized we can take a tight-binding form (6) for the solutions and only keep nearest-neighbor coupling between different n values. For $k=0$ this leads to the set of equations replacing (7),

$$\varepsilon_m a_n+\Delta I_m^{(0)}b_n+\Delta I_m^{(1)}(b_{n-1}+b_{n+1})=Ea_n\,,$$
$$-\varepsilon_m b_n+\Delta I_m^{(0)}a_n+\Delta I_m^{(1)}(a_{n-1}+a_{n+1})=Eb_n\,, \quad (10)$$

where

$$I_m^{(2n-n')}=\int\psi_m^{(n)}f_{n'}\psi_m^{(n'-n)}dx=\frac{m!}{2^{m+1/2}}e^{-(2n-n')^2/\pi}[\exp[-\tfrac{1}{2}(s-t)^2-2(2n-n')\pi^{1/2}(s-t)]]_m \quad (11)$$

where $[\cdots]_m$ means the coefficient of $s^m t^m$ in the expansion of quantity in the bracket. These overlap integrals decrease exponentially with $|2n-n'|$ and the nearest-neighbor approximation is a good one. We can take $u_n,b_n\sim\exp(2\pi i n k_x/q)(-q/2<k_x<q/2)$ and the excitations form bands with energies

$$E_{m,k_x}=\left\{\varepsilon_m^2+\Delta^2\left[I_m^{(0)}+I_m^{(1)}\cos\left(\frac{2\pi k_x}{q}\right)\right]^2\right\}^{1/2}. \quad (12)$$

The bandwidth is of order $\Delta I_m^{(1)}$ and is much smaller than the cyclotron frequency.

We now consider how the qp excitations are modified when $k\neq0$ or $q/2$. It is clear from (4) that for $k\neq0$ the overlap of u_n and v_n is reduced. Supposing k is small, we can take approximate solutions

$$u_n^{(k)}=a\psi_m[x-2l^2(nq+k)]\,,$$
$$v_n^{(k)}=b\psi_m[x-2l^2(nq-k)]\,. \quad (13)$$

Using the same methods as above, it is easily shown that the quasiparticle energies are now

$$E_{m,k_x,k}=\left\{\varepsilon_m^2+\Delta^2\left[I_m\left(\frac{2k}{q}\right)+I_m^1\cos\left(\frac{2\pi k_x}{q}\right)\right]^2\right\}^{1/2}, \tag{14}$$

where

$$I_m(2k/q)=\frac{m!}{2^{m+1/2}}e^{-4\pi k^2/q^2}\times\{\exp[\tfrac{1}{2}(s-t)^2-rk/q(s-t)]\}_m . \tag{15}$$

Thus for $k\neq 0$ the energy gap is reduced by the factor $\exp(-4\pi k^2/q^2)$ and the quasiparticles are approximately electrons or holes. A similar result to (14) applies when $k\sim q/2$ except that $I_m(2k/q)$ is replaced by $I_m(1-2k/q)$.

To summarize, we have obtained the following picture for the excitations outside the vortex cores. The quasiparticle energies fall into bands labeled by the Landau level m. Within each band m, the states are labeled by k_x and, k with $-q/2<k_x$, $k<q/2$ (and k_z in $d=3$) and the energy only depends very weakly on k_x and k through the energy gap Δ^2. The bands have a width Δ and are thus almost flat and separated by ω_c. The number of states in a band is $2L^2/2\pi l^2=2L^2H/\phi_0$, where L^2 is the area of the metal and the 2 in the numerator comes from spin. This is twice the number for a Landau level in a normal metal because the flux quantum in the superconductor is $\phi_0=2\pi c/2e$. At lower fields $H\sim H_{c1}$ this picture is modified. Again suppose that we have a square flux lattice with a spacing d between the vortices so that $Hd^2=\phi_0$. Owing to the lattice periodicity we again expect energy bands with the number of states per band (including spin) to be $2L^2/d^2=2L^2H/\phi_0$. The order parameter $\Delta\sim k_F/m_e\xi$ is now much larger than the magnetic energy $\omega_c\sim 1/m_ed^2$ for high K materials. (The opposite is true near H_{c2}.) In this case for the quasiparticle states above the gap, it is appropriate to start with a free-electron picture and treat the periodic magnetic field and variations in Δ as a perturbation. For high-K materials, Δ is constant except in regions of dimension ξ which we neglect. We suppose that the flux lattice is formed by superposing flux lines at the positions $\boldsymbol{\rho}_{mn}=(md,nd)$. In a gauge in which Δ is real, the vector potential due to a vortex at the origin is

$$\mathbf{A}=\lambda^2\mathrm{curl}\mathbf{H}=\frac{\phi_0}{2\pi\lambda\rho}K_0'(\rho/\lambda)(-y,x), \tag{16}$$

where λ is the penetration depth and K is a Bessel function. We want to solve the Bogoliubov equations (1) with this vector potential in each cell. Of greatest interest are the band gaps which form at the zone boundaries. To estimate these, as discussed above, we begin with a free-quasiparticle picture and treat the vector-potential terms in (1) as a perturbation. Δ is taken to be real and constant. The unperturbed solutions of (1) are then of the usual BCS form

$$\psi_k=\begin{pmatrix}u_k\\ v_k\end{pmatrix}\frac{e^{i\mathbf{k}\cdot\boldsymbol{\rho}}}{\sqrt{L}},\quad \begin{pmatrix}u_k^2\\ v_k^2\end{pmatrix}=\frac{1}{2}\left(1\mp\frac{\varepsilon_k}{E_k}\right) \tag{17}$$

with $\varepsilon_k=k^2/2m_e-\varepsilon_F$ and $E_k=(\varepsilon_k^2+\Delta^2)^{1/2}$. The band gaps occur when $\mathbf{k}=\mathbf{G}/2$ where $\mathbf{G}=(n_x,n_y)2\pi/d$ is a reciprocal lattice vector. To a first approximation, the band gap is

$$\delta_{\mathbf{G}}=|\langle\psi_{-G/2}|\hat{\mathcal{H}}'|\psi_{G/2}\rangle| \tag{18}$$

where

$$\hat{\mathcal{H}}'=\begin{pmatrix}\mathcal{H}' & 0\\ 0 & \mathcal{H}'^*\end{pmatrix},\quad \mathcal{H}'=\frac{e}{m_ec}\mathbf{A}\cdot\mathbf{p}+\frac{e^2}{2m_ec^2}A^2. \tag{19}$$

The terms linear in A give zero and we find

$$\delta_G=\frac{\pi}{4m_e\lambda^2d^2}\left|\frac{\varepsilon_{G/2}}{E_{G/2}}\right|\left|\int_{\mathrm{cell}}d^2\rho e^{i\mathbf{G}\cdot\boldsymbol{\rho}}K_0'^2d^2\right|. \tag{20}$$

If we approximate the unit cell by a circle of radius $d<\lambda$ and cut off the integral at the lower limit $\rho=\xi$ we find

$$\delta_G\simeq\frac{\pi}{4m_ed^2}\left|\frac{\varepsilon_{G/2}}{E_{G/2}}\right||\ln G\xi| . \tag{21}$$

This gap is of order ω_c, the cyclotron frequency, and decreases as the reciprocal lattice vector $\mathbf{G}$ increases. The band gaps are thus similar to those found near H_{c2}. The bandwidths are of order k_F/md and larger than the gaps.

We now discuss some consequences of these results. As the quasiparticles near H_{c2} have a structure similar to the Landau-level structure of electrons in a uniform field, we would expect the quasiparticle magnetization to exhibit de Haas–van Alphen-like oscillations. Because the spacing of the levels (9) is determined by the cyclotron frequency $\omega_c=eH/mc$ the period will be the same as in a normal metal. In order to calculate the oscillating part of the free energy due to the quasiparticles we approximate (14) by $E_m=(\varepsilon_m^2+\Delta^2I_m^2)^{1/2}$, i.e., neglect the variation of the gap with k_x and k. For large m, $I_m\sim 1/(2\pi m)^{1/2}$ and the gap gets small which has an important effect on the amplitude of the de Haas–van Alphen oscillations.[15] In the $d=2$ case the quasiparticle contribution to the free energy per unit area is

$$F=\frac{1}{2\pi l^2}\sum_m\left[\varepsilon_m-\frac{2}{\beta}\ln\left(2\cosh\frac{\beta E_m}{2}\right)\right], \tag{22}$$

where $\beta=1/kT$. Using the Poisson summation formula[16] the oscillating part of F is

$$F_{\mathrm{osc}}=\frac{\omega_c}{8\pi^3l^2}\sum_{p=1}^{\infty}\frac{(-1)^p}{p^2}I(\rho)\cos\frac{2\pi p\varepsilon_F}{\omega_c}, \tag{23}$$

where

$$I(p)=\beta\int_{-\infty}^{\infty}d\varepsilon\exp\left[\frac{2\pi ip\varepsilon}{\omega_c}\right]\left[\frac{1}{\cosh^2\beta E/2}\left[\frac{\partial E}{\partial\varepsilon}\right]^2+\frac{2}{\beta}\tanh\left[\frac{\beta E}{2}\right]\frac{\partial^2 E}{\partial\varepsilon^2}\right]$$
$$=4\exp[-2\pi p\Delta/(\varepsilon_F\omega_c)^{1/2}]f\left[\frac{2\pi p\Delta}{(\varepsilon_F\omega_c)^{1/2}}\right],\ \beta\Delta>1 \qquad (24)$$
$$=\frac{8\pi^2 p/\beta\omega_c}{\sinh(2\pi^2 p/\beta\omega_c)},\ \beta\Delta<1\ ,$$

where $f(0)=1$ and $f(x)=(\pi x/2)^{1/2}x\gg 1$. $F_{\rm osc}$ is of the same form as in a normal metal but the effect of the gap is to reduce the amplitudes in the case where $\beta\Delta>1$. This effect is quite small because the gap is small in the high Landau levels. Thus the quasiparticle magnetization in the mixed state exhibits oscillations with amplitude decreasing with increasing Δ.

We have assumed that the order parameter is of the Abrikosov form (2). Actually, we should make a self-consistent calculation of the order parameter from the quasiparticle spectrum

$$\Delta(r)=g\sum_\alpha u_\alpha v_\alpha^*[1-2f(E_\alpha)]\ , \qquad (25)$$

where α labels the qp states (including those in the core of the vortex lines). From this formula we see that the main contribution to the pairing near H_{c2} comes from states near the band edges $k=0,q/2$ where both u and v are simultaneously large. The self-consistent order parameter contains contributions from all the Landau levels (9) and will thus have a more complicated structure than the Abrikosov form which only includes the lowest Landau level. The lowest level will dominate at sufficiently high fields. A more complicated form for Δ than (2) will not have much effect on our results.

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