de Haas–van Alphen Effect in Anisotropic Superconductors in Magnetic Fields Well Below H_{c2}

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We develop a quasiclassical approach to the energy spectrum of an anisotropic superconductor in a magnetic field, B, such that $H_{c1} \ll B \ll H_{c2}$. Low temperature de Haas–van Alphen oscillations are considered for two cases: (1) the extremal electron orbit may coincide with a symmetry *line* and (2) the orbit crosses *points* where the superconducting order parameter has zeros. The signal is shown to be small in both cases. [S0031-9007(98)05873-6]

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The de Haas–van Alphen (dHvA) effect in superconductors continues to attract theoretical and experimental efforts since its observation in Nb_2Se at fields B below the critical field H_{c2} [1]. The effect was later seen in V_3Si, Nb_3Ge, and borocarbides, for which $H_{c2}(T = 0)$ is high enough to satisfy the criterion $\omega_c\tau \gg 1$ (see [2] for recent review). Theoretical efforts [3–9] have mostly been concentrated on the field range $H_{c2} - B \ll H_{c2}$. Nonzero dHvA effect is considered to be due to a finite normal density of states at the Fermi level, which survives below H_{c2}.

The normal dHvA effect is a quasiclassical feature: the total number of states occupied by electrons in the magnetic field being large, $N \simeq \frac{\mu}{\omega_c} \gg 1$, a minor field variation $\frac{\Delta B}{B} \sim \frac{\omega_c}{\mu}$ leads to crossing the chemical potential by a single level and changing the magnetization in a steplike manner.

We investigate the possibility of a low temperature dHvA for a superconductor in the field regime $H_{c1} \ll B \ll H_{c2}$, where distance between vortices d is large enough to separately treat the "bulk" of the superconductor, where the gap value, $|\Delta(\mathbf{r})|$, is a constant, and the vortex cores, occupying only a fraction, $(\xi_0/d)^2 \ll 1$, of the volume, and their contribution to the dHvA may be neglected. Unfortunately, no experiments have been performed so far in this fundamentally important field range due to limitations imposed by sensitivity of the current experimental methods.

The singularity of the isotropic BCS model at $E = |\Delta|$ results in an exponential reduction of the dHvA amplitude [7]. This might change if superconductivity is anisotropic or the gap has zeros at some symmetry points or on lines along the Fermi surface. For the latter case if the extremal electron trajectory coincides with a zero-gap line, one may expect an increase in the dHvA signal for the corresponding field direction [10]. Another case is "d-wave" superconductivity, now commonly assumed in high T_c cuprates. Here the gap crosses zero at some symmetry *points* of the (2D) Fermi surface. This fact is known [11] to give rise to a finite density of states in the magnetic field at the chemical potential.

We investigated the problem for two situations mentioned above. Our conclusion in the first case is that the dHvA in the regime, $H_{c1} < B < H_{c2}$, is suppressed by the electron's scattering on periodic superconducting currents in the vortex state, leading to Dingle's temperature of order of $\Delta(\xi_0/d)$. The excitation spectrum in the second situation possesses a topologic property which excludes level crossing the chemical potential.

We developed below the approach which allows a general treatment of a superconductor in the mixed state.

In the chosen field range the spatial dependence of the gap is of the form

$$\Delta(\mathbf{r}) = \Delta e^{i\phi(\mathbf{r})}. \tag{1}$$

Superconducting currents outside the vortex cores are

$$\mathbf{j}(\mathbf{r}) = -\frac{c}{4\pi}\,\delta_L^{-2}\left(\mathbf{A} - \frac{c}{2e}\,\nabla\boldsymbol{\phi}\right) \equiv -\frac{c}{4\pi}\,\delta_L^{-2}\mathbf{Q}\,. \tag{2}$$

The topological singularity of the phase at each point, $\mathbf{r}_i$, where the gap passes through zero, results in the following equations [12]:

$$\begin{aligned} \mathrm{curl}\mathbf{Q} &= \mathbf{B} - \boldsymbol{\phi}_0 \sum_i \delta(\mathbf{r} - \mathbf{r}_i)\,, \\ \mathbf{B} - \delta_L^2 \Delta\mathbf{B} &= \boldsymbol{\phi}_0 \sum_i \delta(\mathbf{r} - \mathbf{r}_i)\,. \end{aligned} \tag{3}$$

For the square lattice [$\mathbf{r}_i = d(n, m)$],

$$B(\mathbf{r}) = \frac{\phi_0}{d^2} \sum_{\mathbf{k}} \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\mathbf{k}^2\delta_L^2 + 1}\,; \qquad \left(\mathbf{k} = \frac{2\pi}{d}\,(l, k)\right). \tag{4}$$

From (2) and (4) it follows that

$$\bar{B} = \phi_o d^{-2}, \quad |\mathbf{Q}| \sim \phi_0/d; \quad \Delta B \sim \bar{B}(d/\delta_L)^2, \tag{5}$$

where $B = \bar{B}$ is the spatial field average, and ΔB the weak deviation of B from $\bar{B}$. For simplicity we assume two dimensionality of the Fermi surface.

Quite generally, the oscillatory part of the magnetization M is contained in the expression

$$M = -\frac{\mu}{B}\,\mathrm{Spur}\left(T \sum_{z=i(2n+1)\pi T} G_{11}(z)\right). \tag{6}$$

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Spur$(\cdots)$ means trace over all states (including spin variables) of the component $G_{11}(z)$ of the matrix

$$\hat{G}(z) = \begin{Vmatrix} \mathcal{G}(z) & \mathcal{F}(z) \\ \mathcal{F}^{+}(z) & -\bar{\mathcal{G}}(z) \end{Vmatrix}, \tag{7}$$

which satisfies the system of the Gor'kov equations,

$$\begin{pmatrix} z - (\hat{H} - \mu) & \Delta \\ -\Delta & -z - (\hat{\bar{H}} - \mu) \end{pmatrix} \hat{G}(z) = \hat{1}. \tag{8}$$

In (8) the spatial gap dependence (1), of the phase $\phi(\mathbf{r})$, is removed by an appropriate gauge transformation. On the other hand, the gap itself, $\Delta \equiv \Delta(\mathbf{p})$, may be anisotropic and depend on the position along the Fermi surface.

For simplicity we consider a spherical Fermi surface. Two Hamiltonians $\hat{H}$ and $\hat{\bar{H}}$ in Eq. (8) act on operators $\hat{\psi}$ and $\hat{\psi}^{+}$ in the definitions of the Green function, $\mathcal{G}(z)$ and $\mathcal{F}^{+}(z)$. In a magnetic field they are

$$\hat{\bar{H}}, \hat{H} = \frac{1}{2m}\left(\hat{\mathbf{p}} \pm \frac{e}{c}\mathbf{A}(\mathbf{r})\right)^2. \tag{9}$$

Equations (3) and (4) properly determine the magnetic field outside the cores and the part of the vector $\mathbf{A}(\mathbf{r})$ [or $\mathbf{Q}(\mathbf{r})$] responsible for the periodic variations, leaving unspecified the potential $\mathbf{A}_0(\mathbf{r})$ which corresponds to the average field, $\bar{B} = \mathrm{curl}\mathbf{A}_0(\mathbf{r})$. We write for $\mathbf{A}(\mathbf{r})$ in (9)

$$\mathbf{A}(\mathbf{r}) = \mathbf{A}_0(\mathbf{r}) + \mathbf{Q}(\mathbf{r}) \tag{10}$$

and use below the Landau gauge $\mathbf{A}_{x0} = -\bar{B}y$. [A different choice of $\mathbf{A}_0(\mathbf{r})$ would redefine $\mathbf{Q}(\mathbf{r})$ without affecting its topological singularities in (3).] Expanding in (9)

$$\hat{\bar{H}}, \hat{H} \simeq \frac{1}{2m}\left(\hat{\mathbf{p}} \pm \frac{e}{c}\mathbf{A}_0(\mathbf{r})\right)^2 \pm \frac{e}{c}\hat{\mathbf{v}}_F \cdot \mathbf{Q}(\mathbf{r}) \tag{11}$$

to first order in $\mathbf{Q}$, comparing the linear term with the order of magnitude of the gap in (8), it follows from (5)

$$|(ev_F/c)Q| \sim v_F/d \ll \Delta; \qquad (d \gg \xi_0). \tag{12}$$

To start with, we omit the Q term in (11). In the Landau gauge p_x is conserved. This is also true for Eqs. (8), for the gap couples together momenta p_x and $-p_x$. After p_x is excluded, we have

$$\hat{\bar{H}}, \hat{H} \simeq \frac{1}{2m}\{\hat{p}_x^2 + \hat{p}_y^2\} \pm \frac{e}{mc}(\hat{p}_x\mathbf{Q}_x + \hat{p}_y\mathbf{Q}_y), \tag{13}$$

where $\hat{p}_x, \hat{p}_y$ are the kinetic momenta operators, $[\hat{p}_x, \hat{p}_y] = ie/c\bar{B}$. Here and below all calculations were done in the momentum representation. Correspondingly,

$$\hat{A}_{0x} = -i\bar{B}(d/dp_y). \tag{14}$$

The bare Hamiltonian, $\frac{1}{2m}(\hat{p}_x^2 + \hat{p}_y^2)$, has eigenvalues $E_n = \omega_c(N + \frac{1}{2})$, with real wave functions, which may be used for calculating Spur$\{\cdots\}$ in Eq. (6). The terms linear in $\mathbf{Q}$ in (13), and the gap terms in (8) both result in nondiagonal transitions between free-electron eigenstates for the matrix $\hat{\mathcal{G}}(z)_{N,\bar{N}}$ of the form

$$\sum_{N'} \Delta_{N,N'}\mathcal{F}^{+}_{N'\bar{N}}, \qquad \sum_{N'} \Delta_{N,N'}\mathcal{G}_{N'\bar{N}}, \tag{15}$$

if $\Delta(\mathbf{p})$ is anisotropic.

In the weak coupling limit the gap dependence on distance to the Fermi surface may be neglected. Only the angular dependence of the gap, $\Delta(\mathbf{p})$, on position of the electron momenta along the Fermi surface is relevant. For instance, for d-wave gap, $\Delta^{(d)} \propto p_x^2 - p_y^2$, one has

$$\Delta^{(d)}(\mathbf{p}) = \Delta_0 \cos 2\varphi \equiv \Delta_0(1 - 2p_y^2/p_F^2). \tag{16}$$

The only nonzero matrix elements of operator $\hat{p}_y$ are

$$(\hat{p}_y)_{N,N-1} = (\hat{p}_y)_{N-1,N} = \sqrt{Ne\bar{B}/2c}. \tag{17}$$

One immediately obtains

$$[\Delta^{(d)}(\mathbf{p})]_{N,N\pm2} = (1/2)\Delta_0. \tag{18}$$

[The diagonal elements are zero, as expected from the broken gap symmetry in (16). We have previously used the fact that at the Fermi surface $N \approx p_F^2/2m\omega_c$.]

From (17) and (18) it is straightforward to conclude that the matrix elements, $\Delta_{N,N'}$, in (15), for arbitrary gap anisotropy are of the form

$$\Delta_{N,N'} \equiv \Delta_{N-N'}. \tag{19}$$

Equation (8) then becomes

$$\sum_{N'} \begin{pmatrix} [z - \omega_c(N + \frac{1}{2}) + \mu]\delta_{N',0}; & \Delta_{N'} \\ -\Delta_{N'}; & [-z - \omega_c(N + \frac{1}{2}) + \mu]\delta_{N',0} \end{pmatrix} \hat{G}_{N-N',\bar{N}}(z) = (\hat{1})_{N,\bar{N}}. \tag{8'}$$

Introducing the notation for the chemical potential

$$\mu = \omega_c N_0 + \bar{\mu}, \tag{20}$$

where N_0 is the integer part of μ/ω_c, one may rewrite (8′) for any function f participating in (8′), in the new representation

$$f(\varphi) = \sum_n e^{-in\varphi} f_n; \qquad f_n = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{in\varphi} f(\varphi)\, d\varphi, \tag{21}$$

with $n = N - N_0$ in (8′). As a result, one arrives at the following system of equations:

$$\begin{pmatrix} z - i\omega_c\frac{d}{d\varphi} + \bar{\mu} & \Delta(\varphi) \\ -\Delta(\varphi) & -z - i\omega_c\frac{d}{d\varphi} + \bar{\mu} \end{pmatrix} \hat{G}(z;\varphi,\varphi') = \delta(\varphi - \varphi'), \tag{22}$$

with the periodicity, $f(\varphi + 2\pi) = f(\varphi)$, imposed as the boundary condition. The new Gor'kov's matrix $\hat{G}(z;\varphi,\varphi')$ can be written in the obvious form,

$$\hat{G}(z;\varphi,\varphi') = \sum_{\lambda} \frac{1}{z - E_\lambda} \begin{pmatrix} u_\lambda(\varphi) \\ v_\lambda(\varphi) \end{pmatrix} \otimes (u^*_\lambda(\varphi'), v^*_\lambda(\varphi')), \tag{23}$$

where the BCS notations are adopted for the normalized eigenfunction $[u_\lambda(\varphi), v_\lambda(\varphi)]$. In (23) E_λ is the energy of the level λ with respect to the chemical potential. The eigenvalue problem for the (u, v) functions becomes

$$\begin{aligned} (E - i\omega_c \tfrac{d}{d\varphi} + \bar{\mu}) u(\varphi) + \Delta(\varphi) v(\varphi) = 0, \\ (E + i\omega_c \tfrac{d}{d\varphi} - \bar{\mu}) v(\varphi) + \Delta(\varphi) u(\varphi) = 0, \end{aligned} \tag{24}$$

where (u, v) must be periodic at $\varphi \to \varphi + 2\pi$, as in Eq. (21). Degeneracy of each level remains the same as for free electrons in the magnetic field $\bar{B}$ (per spin; V is the total volume),

$$Ve\bar{B}dp_z/(2\pi)^2 c\,. \tag{25}$$

The expression (6) may be rewritten as

$$M = -\frac{\mu e}{2\pi c} \sum_{\lambda,\sigma} [\overline{|u_\lambda(\varphi)|^2}] n(E_\lambda), \tag{6'}$$

where again we omitted dependence on p_z. Summation in λ runs over all new eigenvalues E_λ. As for the spin energy, it is always small compared to other scales below.

Equations (24) get simpler if we remove $\bar{\mu}$,

$$(u, v) \to e^{-i(\bar{\mu}/\omega_c)\varphi} (\bar{u}, \bar{v}), \tag{26'}$$

and come over to the functions (y, z),

$$\bar{u} = 1/2(y - iz); \qquad \bar{v} = 1/2(z - iy), \tag{26}$$

in terms of which the problem (25) reduces to the Schrödinger equation,

$$E^2 y = -\omega_c^2 y'' + [\Delta^2(\varphi) - \omega_c \Delta'(\varphi)] y, \tag{27}$$

$$z = -\frac{1}{E}[(\omega_c y' + \Delta(\varphi) y], \tag{28}$$

which describes global features for motion of a quasiparticle along the Fermi surface in the magnetic field $\bar{B}$. In particular, at $|E| < \Delta_0$ in (16) excitations are confined in the four "potential wells" formed by $\Delta^2(\varphi)$ around the points $\varphi_k = \frac{\pi}{4} + k\frac{\pi}{4}$. The low energy part ($E \ll \Delta$) of the spectrum is given by the two branches

$$E_n = \pm 2\sqrt{\omega_c \Delta_0 n}; \qquad n = 0, 1, \ldots. \tag{29}$$

It is clear that (29) is not applicable at too low energy E_n because the energy scale $(\omega_c \Delta_0)^{1/2}$ is small, if compared to the $\hat{Q}$ terms in Eq. (11):

$$(d/v_F)(\omega_c \Delta_0)^{1/2} \sim (p_F \xi_0)^{-1/2} \ll 1. \tag{30}$$

To incorporate the Q terms into the scheme of Eqs. (22) and (24) we apply the quasiclassical approach developed in [13]. Omitting details of the derivation, the resulting equation can be obtained from (22) and (24) by the substitution

$$E \Rightarrow E + h(\varphi) \equiv E + (e/c)\mathbf{v}_F \cdot \mathbf{Q}(\mathbf{r}). \tag{31}$$

The dependence on φ is determined by the classical motion of an electron along a circular orbit with the Larmour radius, $r_L = v_F/\omega_c$,

$$\hat{\mathbf{r}} \to \mathbf{r}_0 + (-r_L \cos\omega_c t, r_L \sin\omega_c t), \tag{32}$$

and $\mathbf{v}_F = \dot{\mathbf{r}}, \varphi = \omega_c t$. Assuming that the system in the periodic potentials $\Delta(\varphi), h(\varphi)$ is solved, the Green functions must be averaged over all trajectories.

The term with $h(\varphi)$ represents interactions with periodic currents (2), as seen by an electron moving along the circle r_L with the Fermi velocity v_F. Characteristic frequencies of this motion through the currents' lattice are of order of v_F/d, much larger than ω_c. The rapidly oscillating $h(\varphi)$ terms, while being small compared with the overall gap scale, may smear away fine gap features, such as the spectrum (29). These oscillations take place with a change of φ of order of $\delta\varphi \sim (d/r_L) \ll 1$.

Applying the Poisson's summation formula to expression (6'), taking into account that only the narrow vicinity of the Fermi surface, $|\bar{\lambda}| = |\lambda - N_0| \ll N_0$, may contribute to the dHvA effect, the oscillatory part, $M_{\rm osc}$, after integration by parts, may be written in the form

$$M_{\rm osc} = \frac{i\mu e}{(2\pi)^2 c} \left(2\,\mathrm{Re}\left\{ \sum_{k,\sigma} \frac{1}{k} \exp\left[2i\pi k \left(\frac{\mu}{\omega_c} \right) \right] \times \int_{-\infty}^{+\infty} e^{2i\pi k\bar{\lambda}} \frac{d}{d\bar{\lambda}} [\overline{|u_{\bar{\lambda}}|^2} n(E_{\bar{\lambda}})]\, d\bar{\lambda} \right\} \right). \tag{33}$$

Correspondingly, the two terms arising from differentiation of the expression in the bold parentheses, present oscillations due to a level crossing the chemical potential (at $T = 0$),

$$\Rightarrow \int_{-\infty}^{+\infty} e^{2\pi i k\bar{\lambda}} \overline{|u_\lambda|^2} \delta(E_{\bar{\lambda}})\, d\bar{\lambda}, \tag{33'}$$

or a singularity due to a specific structure of the excitations spectrum in the superconducting state,

$$\Rightarrow \int_{-\infty}^{+\infty} e^{2\pi i k\bar{\lambda}} \frac{d}{d\bar{\lambda}} (\overline{|u_{\bar{\lambda}}|^2}) n(E_{\bar{\lambda}})\, d\bar{\lambda}. \tag{33''}$$

Transition from summation over λ to integration in (33) poses the problem of expressing the energy $E_{\bar{\lambda}}$ as a function of the continuous variable $\bar{\lambda}$.

To implement this approach to the two situations discussed, consider first a symmetry *line* of zeros, and the field direction such that the extremal electron orbit would lie on it. In (22) and (24) the gap equals zero identically, so the electron (hole) wave functions are of the form

$$\exp[\pm iS(\varphi)]; \qquad S(\varphi) = \frac{1}{\omega_c} \int_0^{\varphi} [E + h(\varphi')]\, d\varphi'. \tag{34}$$

The eigenvalue problem follows from the periodicity of (34):

$$2\pi\bar{\lambda} = S(2\pi) = \frac{1}{\omega_c}\int_0^{2\pi}[E_\lambda + h(\varphi')]\,d\varphi'. \quad (34')$$

Comparison with (33) and (33′) leads to the relation between the k components of $M_{\rm osc}$ in the superconducting and normal states,

$$M^S_{\rm osc}(k) = M^N_{\rm osc}(k)\left\langle \exp\frac{ik}{\omega_c}\int_0^{2\pi} h(\varphi')\,d\varphi'\right\rangle. \quad (35)$$

The average in (35) is taken over electronic orbits. By making use of (3), (31), and (32), the exponent may be presented as the integral over the orbit area

$$\frac{1}{\omega_c}\int_0^{2\pi} h(\varphi)\,d\varphi = \frac{e}{c}\oint \mathbf{Q}\cdot d\mathbf{l} = (1/2\phi_0) \times \iint\left[\bar{B} - \phi_0\sum_i \delta(\mathbf{r}-\mathbf{r}_i)\right]dS\,. \quad (36)$$

Here, the factor in exponent (35) measures fluctuations in number of fluxes encircled by electronic orbits n_φ. For a periodic vortex lattice we evaluate (36) in terms of the Gaussian distribution for n_φ with the average, $\overline{n_\varphi}$, as

$$\overline{n_\varphi} = (2\pi r_L d)/d^2 = 2\pi(r_L/d)\,. \quad (37)$$

For the Dingle factor, $\exp[-2\pi cm/e\tau\bar{B}]$, we get

$$1/\tau \sim \Delta_0(\xi_0/d)\,. \quad (38)$$

Note that (37) is but an estimate. In any case, the dHvA signal will be very weak: $(\tau\omega_c)^{-1} \sim p_F d \gg 1$.

Turn now to the other case when the orbits of normal electrons would cross points at the Fermi surface where the gap changes sign and passes through zero, as in Eq. (16). Although (29) is not applicable at small n, its structure indicates that the dHvA contribution (33′) is to be zero identically. In fact, the dHvA effect consists in pushing up an energy level through the chemical potential at small field variation. Equation (25) is qualitatively different from the spectrum of normal electrons in that, while in the latter case levels are pushed up from the bottom of the band, d-wave superconductivity *fixes* levels structure in the vicinity of the chemical potential. The (+) and (−) branches in (29) are moving up and down, respectively, with the field increase. The existence of levels in the vicinity of $E = 0$ is a topological property for a solitonlike problem [14] at each point $\varphi_k = \frac{\pi}{4} + k\frac{\pi}{2}$, where (16) changes its sign. We argue that superconducting currents (31) only randomize the spectrum (29) without a change in the above physics.

Consider the limiting case when $\Delta(\varphi)$ changes sign in a steplike manner [14]:

$$\Delta(\varphi) = \Delta\,\mathrm{sgn}(\varphi - \varphi_k)\,. \quad (39)$$

Equation (27) becomes the familiar Schrödinger equation with the δ-function potential. There is only one bound state (for each φ_k) which lies exactly at $E = 0$ (neglecting a weak overlap between points). The wave function exponentially decays at $|\varphi - \varphi_k| > \omega_c/\Delta$, on which scale variation of $h(\varphi)$ is negligible. For a given trajectory, hence, the position of such a level is shifted: $E = -h(\varphi_k)$. Thus, levels close to the chemical potential remain separated from the manifold of levels $E^2 > \Delta^2$. Their dependence on magnetic field $\bar{B}$ shows up through dependence of $|h| \sim v_F/d \sim \bar{B}^{1/2}$, i.e., is the same as in (29). Averaging over trajectories smears each level into a band, $|\Delta E| \sim v_F/d$. Recall now that one level has the capacity (25). In the 2D case it produces the density of states of order [15]

$$v^S \sim \frac{e\bar{B}}{c}\frac{d}{v_F} \sim v^N\frac{\Delta}{\varepsilon_F}\left(\frac{\bar{B}}{H_{c2}}\right)^{1/2}.$$

To summarize, we developed a rigorous approach to quantization of motion of superconducting excitations in the presence of magnetic field $\bar{B} \ll H_{c2}$. The dHvA effect is formulated in terms of a singularity produced either by the Fermi function or by a modified structure of levels in the superconducting state. For an order parameter with a line of zeros there is a field direction at which dHvA oscillations may become observable. In case of points of zeros on a 2D Fermi surface the effect is expected to be weaker. Analysis of dHvA effects produced by singularities in the energy spectrum of the superconducting state will be published elsewhere.

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