Gap Anisotropy and de Haas-van Alphen Effect in Type-II Superconductors

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We present a theoretical study on the de Haas-van Alphen (dHvA) oscillation in the vortex state of type-II superconductors, with a special focus on the connection between the gap anisotropy and the oscillation damping. Numerical calculations for three different gap structures clearly indicate that the average gap along the extremal orbit is relevant for the magnitude of the extra damping, thereby providing support for experimental efforts to probe gap anisotropy through the dHvA signal.

We also derive an analytic formula for the extra damping which will be useful to estimate angle- and/or band-dependent gap amplitudes.

A considerable number of materials have been found in the 1990s to exhibit de Haas-van Alphen (dHvA) oscillation in the superconducting vortex state [1], the phenomenon discovered by Graebner and Robbins in 2H-NbSe$_2$ [2]. Many theories have been put forward during the same period to explain this fundamental phenomenon observed in the system without a well-defined Fermi surface [1]. However, there is yet no established theory comparable with the normal-state Lifshitz-Kosevich (LK) theory [3]. Moreover, what is lacking seems to be a clear physical picture of the mechanism of the extra oscillation damping in the vortex state. To improve the situation, we present here a numerical study combined with an analytical one.

Novel aspects in our study are summarized as follows:

(i) We perform three-dimensional numerical calculations for the dHvA oscillations in the vortex state using the Bogoliubov-de Gennes equations. To date, numerical studies have been carried out only for the two-dimensional $s$-wave model, such as that of Norman et al. (NMA) [4]. Our results show that dHvA oscillations in three dimensions are quantitatively different in the vortex state from those in two dimensions.

(ii) To clarify the connection between the oscillation attenuation and the gap anisotropy, we use three different gap structures: $s$-wave, $d$-wave with four point nodes in the extremal orbit, and $p$-wave with a line node in the extremal orbit; see Eq. (2) below. It is thereby shown that the attenuation is determined by the average gap along the extremal orbit in zero magnetic field (see Fig. 1), in disagreement with the theory of Miyake [5]. This result still indicates that one can probe the angle- and/or band-dependent gap amplitude in zero field with the dHvA effect in the vortex state. The origin of the discrepancy from Miyake’s result is discussed in some detail.

(iii) We derive a new analytic formula for the extra Dingle temperature in the vortex state:

$$k_B T_D = 0.5\hat{\Gamma} \langle |\Delta_p|^2 \rangle_{eo} \frac{m_0 c}{\pi e h} \frac{1 - B/H_{c2}}{B}.$$  \hspace{1cm} (1)

Here, $\hat{\Gamma} = 0.125$ is a dimensionless quantity characterizing the Landau-level broadening due to the pair potential, $\langle |\Delta_p|^2 \rangle_{eo}$ denotes the average gap along the extremal orbit in zero field, $m_0$ is the band mass, and $B$ and $H_{c2}$ are the average flux density and the upper critical field, respectively.

Equation (1) is derived below through the second-order perturbation with respect to the pair potential, i.e., an approach from $H_{c2}$, which is useful to estimate the gap amplitude along the extremal orbit. A difference from Maki’s formula [6] lies in the prefactor where the Fermi velocity $v_F$ is absent. Indeed, a dimensional analysis on the second-order perturbation tells us that the Landau-level broadening in the vortex state should be of order $[\Delta^0(B)]^2/\hbar \omega_c$, where $\hbar \omega_c$ is the cyclotron energy and $\Delta^0(B) \propto \sqrt{\langle |\Delta_p|^2 \rangle_{eo}(1 - B/H_{c2})}$ is essentially the average gap along the extremal orbit. This leads to Eq. (1) except for the numerical constant.

Terashima et al. [7] reported a dHvA experiment on YNi$_2$B$_2$C where an oscillation (labeled $\alpha$) is seen to persist down to a field of order $0.2H_{c2}$. On the other hand, a specific-heat experiment at $H = 0$ shows a power-law behavior $\propto T^3$ at low temperatures [8], indicating the existence of the gap anisotropy in this material. This gap anisotropy may also play an important role for the dHvA signal far below $H_{c2}$. By using Eq. (1), the average gap of this band $\alpha$ will be estimated at the end of the paper.

Model: Our starting point is the Bogoliubov-de Gennes equation for the quasiparticle wavefunctions $u_s$ and $v_s^*$ labeled by a quantum number $s$ with a positive eigenvalue $E_s$:

$$\int dr_2 \left[ \begin{array}{c} \mathcal{H}(r_1, r_2) - \Delta(r_1, r_2) \\ -\Delta^*(r_1, r_2) - \mathcal{H}^*(r_1, r_2) \end{array} \right] \left[ \begin{array}{c} u_s(r_2) \\ v_s^*(r_2) \end{array} \right] = E_s \left[ \begin{array}{c} u_s(r_1) \\ -v_s^*(r_1) \end{array} \right].$$  \hspace{1cm} (2)

Here $\Delta$ is the pair potential and $\mathcal{H}$ denotes the normal-state Hamiltonian in the external field $\mathbf{H} \parallel \mathbf{z}$, both are $2 \times 2$ matrices to describe the spin degrees of freedom. We adopt as $\mathcal{H}$ the free-particle Hamiltonian. As for the pair potential, we wish to consider three cases to yield the following energy gaps at $H = 0$:
\( \Delta_p = \begin{cases} 
\Delta_0 W_p i \sigma_y \\
\Delta_0 W_p \sin^2 \theta_p \cos 2 \varphi_p i \sigma_y \\
\Delta_0 W_p \cos \theta_p i \sigma_y 
\end{cases} \),

(3)

where \( p \) is the momentum, \( W_p \) denotes some cut-off function with \( W_p = 1 \) (\( p_p \): Fermi momentum), \( \theta_p \) (\( \varphi_p \)) is the polar (azimuthal) angle, and \( \sigma_y \)'s are the Pauli matrices. The first one is the isotropic \( s \)-wave state, whereas the latter two have four point nodes (\( d \)-wave) and a line node (\( p \)-wave), respectively, in the extremal orbit of the \( xy \) plane perpendicular to \( \mathbf{H} \parallel \mathbf{z} \). It then turns out that the orbital part of the corresponding pair potentials in finite fields can be expanded with respect to \( r \equiv r_1 - r_2 \) and \( \mathbf{R} = \frac{1}{2} (r_1 + r_2) \) as

\[
\Delta(r_1, r_2) = \frac{N_f}{\sqrt{2}} \sum_{N_c} \Delta^{(N_c)}(B) \psi_{N_c, q}(\mathbf{R}_\perp) \sum_{N_{m, p}} (-1)^{N_c} \times \frac{W_p}{W_p} \sin^2 \theta_p \cdot \phi_{\text{ipz}}/h \int_{L_z} \psi_{N_{m, p}}(r_\perp) \frac{W_p \sin^2 \theta_p}{W_p \cos \theta_p} .
\]

(4)

Here \( N_c \) and \( N_r \) denote the Landau levels in the average flux density \( B \), \( q \) is an arbitrarily chosen center-of-mass magnetic Bloch vector, and \( m \) signifies the relative angular momentum along the \( z \) axis so that \( m = 0, 0, \pm 1 \) for the three cases, respectively, in a system with \( N_r^2/2 \) flux quanta and the length \( L_z \) along the \( z \) axis. The arguments \( r_\perp \) and \( \mathbf{R}_\perp \) denote the \( xy \) components, and \( p \) and \( \theta_p \) are to be evaluated at \( p = (p_z^2 + \hbar^2 N_r/l_B^2)^{1/2} \) and \( \theta_p = \tan^{-1} \frac{\hbar \sqrt{N_r/l_B}}{p_z} \) with \( l_B = (\hbar c/eB)^{1/2} \). See ref. \( 3 \) for the expressions of the basis functions \( \psi_{N_c, q} \) and \( \psi_{N_{m, p}} \).

A significant advantage of Eq. (2) is that the coefficients \( \{ \Delta^{(N_c)} \}_{N_c=0} \) completely specify the pair potential, and the first few terms suffice to describe those of \( B \gtrsim 0.1 H_{c2} \). The self-consistent mean-field theory \( 1, 3 \) predicts an oscillatory reentrant behavior of \( H_{c2} \) and \( \Delta^{(N_c)} \). On the contrary, such a singular behavior of \( H_{c2} \) has never been identified definitely in any materials displaying the dHvA oscillation in the vortex state. Leaving the puzzling discrepancy for a future study, we here adopt the quasiclassical \( \Delta^{(N_c)} \) rather than the fully self-consistent one, with the square-root behavior

\[
\Delta^{(0)} \equiv a(1 - B/H_{c2})^{1/2}
\]

(5)
of the mean-field second-order transition for the dominant \( N_c = 0 \) level. Then the best choice for \( \{ \Delta^{(N_c)} \}_{N_c=0} \) would be to use the results from the Eilenberger equations. Since our main interest lies in studying the differences in the oscillation damping among various gap structures, however, we here adopt a model form of \( \Delta^{(N_c)} \) determined by requiring that the maximum of \( \frac{1}{V} \int d\mathbf{R} \left| \int d\mathbf{r} \Delta \Delta (r_1, r_2) e^{-i \mathbf{p} \cdot \mathbf{r}/\hbar} \right|^2 \) be equal to \( \Delta_0^2 (1 - B/H_{c2}) \), where \( V \) is the volume of the system and \( \Delta_0 \) denotes the maximum energy gap of the weak-coupling theory at

\[
T = H = 0.
\]

This is possible within the lowest-Landau-level approximation of retaining only \( \Delta^{(0)} \), which is excellent for \( B \gtrsim 0.1 H_{c2} \). The resulting \( \Delta^{(0)} \) also displays the square-root behavior, and our numerical calculation shows that \( a^2 \approx 0.5 \Delta_0^2 \) in all the three cases. We are planning to report on the best choice for \( a \) from the Eilenberger equations.

The use of the quasiclassical pair potential \( 1 \) has an advantage: Self-consistent calculations for the continuum model \( 3 \) necessarily result in a rather small number of Landau levels below the Fermi energy \( \varepsilon_F \), i.e., \( N_F \sim 10 \) at \( H_{c2} \), hence failing to meet the condition \( N_F \gg 1 \) appropriate for real materials. The present calculation with Eq. (3) is free from such a limitation. We have performed calculations including about 50 Landau levels below \( \varepsilon_F \) for the extremal orbit at \( H_{c2} \).

Since the relevant materials have large Ginzburg-Landau parameter \( \kappa \gg 1 \), we also neglect the screening in the magnetic field. Indeed, the effect has been shown to be irrelevant for the oscillating damping \( 3 \). We put \( T = 0 \), adopt \( W_p = e^{-i(\mathbf{q} \cdot \mathbf{p}/0.1e^2)} \) with \( \mathbf{q} \) the normal-state one-particle energy measured from \( \varepsilon_F \), and choose the cyclotron energy at \( H_{c2} \) as \( h \omega_c = k_B T_c \), in accordance with \( h \omega_{c2}/k_B T_c \sim 1 \) for real materials.

**Numerical Method:** To solve it numerically for the above model, we transform Eq. (2) into the eigenvalue problem for the expansion coefficients of \( \mathbf{u}_s \) and \( \mathbf{v}_s \) in the quasiparticle basis functions \( \{ \psi_{N_\kappa \sigma} \} \), where \( k \) is a quasiparticle magnetic Bloch vector and \( \alpha \) (= 1, 2) signifies twofold degeneracy of the orbital states \( 3 \). Then it can be solved separately for each \( k\sigma \) due to the translational symmetry of the vortex lattice. The overlap integral between \( \psi_{N_\kappa \sigma}^{(e)}(\mathbf{R}_\perp) \psi_{N_\kappa \sigma}^{(r)}(\mathbf{r}_\perp) \) and \( \psi_{N_\kappa k_1 \alpha_1}(\mathbf{r}_\perp) \psi_{N_\kappa k_2 \alpha_2}(\mathbf{r}_\perp) \) vanishes unless \( k = k_1 \) and \( k_2 \) and \( \alpha_1 = \alpha_2 \) so that the calculations are simplified greatly. The corresponding eigenstate is labeled explicitly by \( s = (\kappa \sigma \alpha_1 \sigma) \) with \( \nu \sigma \) the band (spin) index.

**Numerical results:** Figure 1(a) presents the oscillation of the \( s \)-wave magnetization as compared with the normal-state one. We see clearly that the oscillation frequency is unchanged from that of the normal state. With \( h \omega_c = k_B T_c \) at \( H_{c2} \), the oscillation is observed to persist down to a rather low field of \( H_{c2}/B \approx 1.8 \), i.e.,

\[
B \gtrsim 0.55 H_{c2},
\]

which is lower than 0.8 \( H_{c2} \) where \( h \omega_c \) becomes equal to the spatial average of the energy gap: \( \Delta_0 (1 - B/H_{c2})^{1/2} \). This is partly because the gap is smaller within the extremal orbit, as shown by Brandt et al. \( 13 \). The points with error bars in Fig. 1(b) comprise the corresponding Dingle plot for the extra damping factor \( \kappa \) obtained by numerical differentiation. This extra damping at high fields shows the behavior \( \propto 1 - B/H_{c2} \) in the logarithmic scale, but an irregularity sets in around 0.55 \( H_{c2} \) where the oscillation disappears. We attribute this irregularity to the effect of the bound-state formation in the core region. The lines are the predictions from various theoretical formulas. The Maki formula \( 1 \) repro-

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predict rapid attenuation incompatible with our numerical data. Indeed, Miyake obtained his analytic formula by applying a semiclassical quantization condition for the expression of the electron number \( N \) at \( B = 0 \). Neither of his starting point \( N(B = 0) \) nor the use of the quantization condition may be justified for describing the dHvA signals observed mainly near \( H_{c2} \).

In the line-node case of Figs. 1(e) and 1(f), in contrast, we observe a much weaker damping in favor of Miyake’s idea \([5]\). However, the non-zero extra damping can only be explained by considering the contribution of some finite width near the extremal orbit. Using Eq. (1) to obtain the best fit to the numerical data, i.e., the solid line of Fig. 1(f), we estimate that the region \( |p_1| > p_f \sin \frac{\pi}{2} \) contributes to the extra attenuation. This is in rough agreement with the estimation from the Fresnel integral \( \int_{-\infty}^{\infty} \exp[-i(\sqrt{2\pi N_F} p_2/p_f)^2] dp_2 \) which appears in obtaining the LK formula: Cutting the infinite integral at \( \sqrt{2\pi N_F} p_2/p_f \approx 10 \) with \( N_F \approx 50 \) yields a similar value for the relevant range of \( p_2 \).

**Analytic Formula:** The Luttinger-Ward free-energy functional corresponding to Eq. (1) is given by

\[
\Omega = -\frac{k_B T}{2} \sum_n \text{Tr} \ln \left[ \frac{\mathcal{H} - i\varepsilon_n \frac{\mathcal{A}}{2}}{-\mathcal{A}^*} - \frac{\mathcal{A}^* - i\varepsilon_n}{\mathcal{A}} \right] \times \left[ e^{i\varepsilon_n \sigma_+ 1} 0 \right] + \cdots ,
\]

\[(6)\]

where \( \varepsilon_n/\hbar \) is the Matsubara frequency and \( 0_+ \) is an infinitesimal positive constant. The terms \( \cdots \) may be expressed solely with respect to the pair potential so that they can be neglected in the present model to consider the oscillatory part. This \( \Omega \) may be transformed into

\[
\Omega = -\sum_s \left[ k_B T \ln(1+e^{-E_s/k_B T}) + E_s \int |\mathbf{v}_s(\mathbf{r})|^2 d\mathbf{r} \right].
\]

(7)

Since we are interested in the extra damping in the vortex state, we adopt as \( E_s \) and \( \mathbf{v}_s \) the expressions from the second-order perturbation with respect to \( \Delta \). They are

\[
E_{N\kappa\rho_{p_s}} = |\xi_{Np_s}| + (1)_{N\kappa p_s} \text{sign}(\xi_{Np_s}) ,
\]

\[(8)\]

\[
\int |\mathbf{v}_{N\kappa p_{p_s}}(\mathbf{r})|^2 d\mathbf{r} = \theta(-\xi_{Np_s}) + \eta^{(2)}_{N\kappa p_s} \text{sign}(\xi_{Np_s}) ,
\]

\[(9)\]

where \( \theta(\xi) \) is the step function and \( \eta^{(1)}_{Np_s} \equiv \sum_{N'} |\int \psi^*_{N'\kappa p_s}(\mathbf{r}_1) \psi_{N'\kappa -\kappa_0}(\mathbf{r}_2) - \eta^{(1)}_{N'\kappa p_s} \frac{1}{L_z} \Delta(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2 |^2 / (\xi_{N\kappa p_s} + \xi_{N'-\kappa p_s}) \)^n. The first terms on the right-hand

![Fig. 1](attachment:image.png)
side of these equations are just the normal-state expressions. The second terms, on the other hand, denote the finite quasiparticle dispersion in the magnetic Brillouin zone and the smearing of the Fermi surface, respectively, due to the scattering by the growing pair potential. It is useful to express $\eta_{N_{kp}}^{(n)}$ in terms of $\tilde{\Delta}(0)(B)$ and the cyclotron energy $\hbar\omega_c$, of the extremal orbit as

$$\eta_{N_{kp}}^{(n)} = \frac{|\tilde{\Delta}(0)(B)|^2}{(\hbar\omega_c)^n} \tilde{\eta}_{N_{kp}}^{(n)}.$$  \hspace{1cm} (10)

The quantity $\tilde{\eta}_{N_{kp}}^{(n)}$ thus defined is dimensionless, and we realize that the main B dependence in Eq. (10) lies in the prefactor $|\tilde{\Delta}(0)(B)|^2/(\hbar\omega_c)^n$. The explicit expression of $\eta_{N_{kp}}^{(n)}$ is given by

$$\eta_{N_{kp}}^{(n)} = \frac{A^2}{4} \sum_{N'} \left( \langle N'N|0N^+\rangle \langle N+N'+m|2k-q\rangle \right)^2 \times (2k-q|N+N'+m') \times \left\{ \begin{array}{ll} \sin^2 \theta_p, & m'=0,0, \text{ or } \pm 2 \end{array} \right.$$  \hspace{1cm} (11)

where the overlap integrals are given by eqs. (3.23) and (2.9) of ref. [2]. $\delta = \delta(B, p_z)$ ($|\delta| < 1/2$) specifies the location of $E_F$ between the two closest Landau levels, and $m, m' = 0, 0, \pm 2$ for the three cases of Eq. (11), respectively. The corresponding normalized density of states:

$$D_{N_{kp}}(\tilde{\eta}) = \frac{2}{\sqrt{\pi}} \sum_{k\alpha} \delta(\tilde{\eta} - \tilde{\eta}_{N_{kp}}^{(n)}),$$  \hspace{1cm} (12)

will play a central role in the following.

Substituting eqs. (8) and (9) into Eq. (7), we find that

$$\Omega_1 = -\frac{k_B T}{2\pi^2 h^2 B} \int_{-1/2}^{1/2} dN \cos(2\pi N) \int_{-\infty}^{\infty} dp_z \int_{-\infty}^{\infty} d\tilde{\eta} \times D_{N_{kp}}^{(1)}(\tilde{\eta}) \ln \left[ 1 + e^{-\left( \xi_{N_{kp}} + \tilde{\eta} \left| \tilde{\Delta}(0)(B) \right|^2 / (\hbar \omega_c) \right) / k_B T} \right].$$  \hspace{1cm} (13)

The function $D_{N_{kp}}^{(1)}(\tilde{\eta})$ depends on $(N, p_z)$, but may be replaced by a representative one $\tilde{D}_{\ell}(\tilde{\eta})$ to be placed outside the $N$ and $p_z$ integrals [12], where the recovered index $\ell$ specifies the $s$-, $d$-, or $p$-wave case of Eq. (11). It may also be acceptable to use a Lorentzian for it: $\tilde{D}_{\ell}(\tilde{\eta}) = \tilde{\Gamma}_\ell / (\pi(\tilde{\eta}^2 + \tilde{\Gamma}_\ell^2))$ [13]. We thereby obtain an expression for the magnetization which carries an extra damping factor:

$$R_s(B) = \int_{-\infty}^{\infty} \tilde{D}_{\ell}(\tilde{\eta}) \exp \left[ -2\pi i \tilde{\eta} \tilde{\Delta}(0)(B) / (\hbar \omega_c) \right] d\tilde{\eta} = \exp \left[ -2\pi i \tilde{\eta} \tilde{\Delta}(0)(B) / (\hbar \omega_c) \right].$$  \hspace{1cm} (14)

Thus, the superconductivity gives rise to an extra Dingle temperature of $k_B T_\Delta = \tilde{\Gamma}_\ell / (\tilde{\Delta}(0)(B)^2 / (\hbar \omega_c)^2$, or equivalently, the extra scattering rate of $\tau^{-1} = 2\pi k_B T_\Delta / h$.

Equation (14) may have an advantage that one can trace the origin of the extra dHvA damping definitely to the growing pair potential, which brings about a finite quasiparticle dispersion (1) in the magnetic Brillouin zone and the corresponding Landau-level broadening, Eq. (12). Moreover, Eq. (11) reveals that this broadening near $\hbar\epsilon_2$ is closely connected with the zero-field gap structure, Eq. (3).

There seems to be no analytic way to estimate $\tilde{\Gamma}_s$, so we determine it using the best fit to the numerical data of Fig. 1(b). Using Eq. (2) with $a^2 = 0.5\Delta_0^2$, the procedure yields $\tilde{\Gamma} \equiv \tilde{\Gamma}_s = 0.125$, as noted before. It is also clear for the anisotropic cases that the average gap around the extremal orbit is relevant for the extra attenuation, as may be realized from Eq. (11). We hence put $a^2 = 0.5(|\Delta_p|^2)_{\alpha \tilde{\Gamma}_s}$. We thereby obtain Eq. (14), which gives a good fit to the $d$-wave numerical data without any adjustable parameters; see Fig. 1(d).

Concluding Remarks: We have shown explicitly that the dHvA effect in the vortex state can be a powerful tool to probe the average gap along the extremal orbit. Such an experiment has recently been performed on UPd$_2$Al$_3$ by Inada et al. [13], and Eq. (14) will be useful in similar experiments to estimate angle- and/or band-dependent gap amplitudes. Using the $\alpha$ oscillation of YNi$_2$B$_2$C observed by Terashima et al. [14], for example, we obtain $\langle |\Delta_p|^2 \rangle_{\alpha \tilde{\Gamma}_s} = 1.5$meV for this $\alpha$ band, a value much smaller than 2.5meV from the specific-heat measurement [15]. It should be noted, however, that the numerical factor 0.5 in Eq. (14) comes from our model described below Eq. (14). It has to be replaced by the result from the Eilenberger equations. We are planning to report on this together with detailed comparisons with experiments in the near future.

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