

Ginzburg-Landau-Gor'kov theory of magnetic oscillations in a type-II two-dimensional superconductor

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(Received 14 August 1996; revised manuscript received 18 February 1997)

We investigate de Haas–van Alphen (dHvA) oscillations in the mixed state of a type-II two-dimensional superconductor within a self-consistent Gor'kov perturbation scheme. Assuming that the order parameter forms a vortex lattice we can calculate the expansion coefficients exactly to any order. We have tested the results of the perturbation theory to fourth and eighth order against an exact numerical solution of the corresponding Bogoliubov–de Gennes equations. The perturbation theory is found to describe well the onset of superconductivity close to the transition point H_{c2} . Contrary to earlier calculations by other authors we do not find that the perturbative scheme predicts any maximum of the dHvA oscillations below H_{c2} . Instead we obtain a substantial damping of the magnetic oscillations in the mixed state as compared to the normal state. We have examined the effect of an oscillatory chemical potential due to particle conservation and the effect of a finite Zeeman splitting. Furthermore, we have investigated the recently debated issue of the possibility of a sign change of the fundamental harmonic of the magnetic oscillations. Our theory is compared with experiment and we have found good agreement. [S0163-1829(97)03226-8]

I. INTRODUCTION

In recent years there has been a renewed interest in the interplay between external magnetic fields and superconductivity in type-II superconductors. It is well known that de Haas–van Alphen (dHvA) oscillations are a useful tool for probing the Fermi surface in metals in the normal state. For type-II superconductors the magnetic field is allowed to partially penetrate the sample in the mixed state. One would then expect magnetic oscillations in the mixed state to give information about the quasiparticle dispersion and the magnetic field dependence of the correlations in the ground state. Magnetic oscillations in the mixed state were observed for the first time in the layered superconductor 2H-NbSe₂ over 20 years ago.¹ More recently dHvA oscillations were observed in the organic superconductor κ -(ET)₂Cu(NCS)₂,² the A15 compounds V₃Si (Ref. 3) and Nb₃Sn,⁴ the borocarbide superconductor YNi₂B₂C,⁵ and the high-temperature superconductors YBaCuO (Ref. 6) and BaKBiO.⁷ These experiments have sparked a variety of theoretical investigations, not least in order to understand the interplay between oscillations in the quasiparticle spectra and the ground-state condensation energy. The transition line H_{c2} between the normal state and the mixed state was shown to exhibit weak oscillations as a function of the magnetic field.^{8,9} For high magnetic fields, clean samples, and very low temperatures H_{c2} has been predicted theoretically to be a strongly oscillating function.¹⁰ The mixed state is characterized by the interplay between Landau level quantization due to the magnetic field and Cooper pair formation characteristic of superconductivity. This calls for a theory that takes both effects into account consistently. The theory developed by Maki¹¹ and Stephen¹² gives a simple picture of the vortex lattice acting as an extra scattering potential on quasiparticles, thereby damping the magnetic oscillations. The theory uses semiclassical approximations and, crucially, fails to impose

the physical condition that the vortex lattice is the self-consistent mean field of the Cooper pairs. The problem simplifies when the electrons are confined to form pairs within the same Landau level (diagonal approximation) and this case has been treated by several authors.^{13,14} Unfortunately the diagonal approximation ignores the fact that the typical excitation is a superposition of an electron and a hole in different Landau levels, but with similar energies. This effect is strongest when the chemical potential μ is either at a Landau level $n_f = \mu/\hbar\omega_c - 1/2 = n$ (n integer) or exactly between two Landau levels $n_f = n + 1/2$. We then have exact degeneracy between an electron state in a Landau level $n_f + m$ and a hole in the level $n_f - m$, when $n_f = n$, and between an electron in a level $n_f + m + 1/2$ and a hole in a level $n_f - m - 1/2$, when $n_f = n + 1/2$, respectively. A major effect of the self-consistent pairing field is then to mix these two degenerate excitations strongly. Following the results of the diagonal approximation Dukan and Tešanović¹⁵ have focused on the consequences of a gapless portion of the quasiparticle spectrum. The calculation, which is appropriate for low-lying excitations in three dimensions, is not applicable for two-dimensional (2D) systems where the number of gapless points and their dispersion law vary strongly with the magnetic field and it does not take into account the oscillatory behavior of the ground-state energy as a function of the magnetic field. This oscillatory behavior of the ground-state energy has been considered by Miller and Györfy¹⁶ in the $\Delta \gg k_B T$ limit. Norman *et al.*¹⁷ have studied the problem numerically and have linked the damping of the magnetic oscillations to the broadening of the Landau levels due to the gap. Recently¹⁸ there have been claims based partly on Gor'kov theory and partly on an assumed simplified form for the quasiparticle spectrum that below a certain field $H_{inv} < H_{c2}$, the magnetic oscillations should exhibit a rapid 180° phase shift.

In this paper we develop a scheme for calculating the

Gor'kov expansion terms treating the quantum effects of the magnetic field exactly. In addition we solve numerically the corresponding Bogoliubov–de Gennes (BdG) equations. Using the developed formalism we study the magnetic oscillations in the mixed state of a type-II superconductor. We are working in two dimensions since many organic metals are known to show almost perfect 2D behavior. Exploiting the symmetry of the magnetic translation group of the vortex lattice we have been able to calculate the expansion coefficients in the Gor'kov theory exactly to any order, making no restriction on the energy of the center of mass of the Cooper pairs. Self-consistency within this approach then transforms to the much simpler problem of minimizing a polynomial of a finite number of variables. This allows us to develop an analytical theory for the thermodynamic potential and thus for the magnetic oscillations close to H_{c2} which contains no approximations apart from the assumption of a small order parameter. This establishes a rigorous basis for our theory, compared with earlier attempts. It turns out to be crucial to determine the order parameter self-consistently since its oscillatory behavior when the magnetic field varies is the cause of the damping of the dHvA oscillations. We find that the dHvA oscillations are damped in the mixed state as compared to the normal state, in agreement with what is observed experimentally. This is due to the fact that the contribution from the superconducting order parameter to the magnetic oscillations partly cancels the contribution from the normal grand potential. The superconducting order parameter itself is an oscillating function of the magnetic field, with local maxima occurring whenever we have a Landau level at the chemical potential since electrons can then form Cooper pairs without any cost in kinetic energy. This is the simple physical picture of the damping emerging from our formalism and it complements the interpretation given by Miller and Györfy¹⁶ and Norman *et al.*¹⁷ When many Landau levels participate in the pairing we have simplified the expressions for the expansion parameters. This makes it possible to give fairly simple analytical expressions for the rate of damping of the dHvA oscillations close to the transition line that may prove useful when fitting experimental data.

A similar approach has been taken by Maniv *et al.*¹⁹ Using the semiclassical and various other approximations, they calculate the Gor'kov expansion coefficients for a 2D metal to fourth order in $\Delta(\mathbf{r})$ when the motion of the centers of mass of the Cooper pairs is restricted to the lowest Landau level. However, they obtain²⁰ that the magnitude of the magnetic oscillations exhibit a maximum below H_{c2} . This is contradicted by our exact calculation of the expansion coefficients and also by our numerical solution to the BdG equations.

Recently it has been suggested that the degeneracy of the Landau levels should give rise to nonperturbative terms in the expansion of the grand potential, thereby making the traditional Gor'kov theory invalid.²¹ We have tested our perturbative theory carefully against an exact numerical solution of the BdG equations and we do not find any of the predicted nonperturbative effects. The theory based on the Gor'kov expansion agrees very well with the exact solution if we are not too far below H_{c2} . It is essentially a high-temperature expansion in the sense that is an asymptotic series as long as the change in the quasiparticle levels as compared to the

normal state is not larger than $\sim O(k_B T)$.²²

In a two-dimensional metal the chemical potential is an oscillatory function of the magnetic field when the number of particles N is fixed. When higher harmonics are important (i.e., low temperatures and clean samples) the dHvA signal in the normal state for fixed N looks qualitatively different from the case when the chemical potential is fixed. It is of interest to see what consequences this difference has for the magnetic oscillations in the mixed state. Examination of the dHvA oscillations in the mixed state in the two cases yields that the superconducting order for fixed number of particles reduces the oscillations in the chemical potential and that the dHvA oscillations are essentially the same in the two cases apart from a narrow region close to H_{c2} . Specifically, the rate of damping of the magnetic oscillations is the same when the number of particles is constant and when the chemical potential is constant.

Since the contribution to the magnetic oscillations from the condensation energy is in antiphase with the contribution from the normal grand potential, it has been suggested¹⁸ that this will result in a sign change of the fundamental harmonic of the dHvA oscillations for $H \leq H_{\text{inv}} < H_{c2}$. This would happen if the superconducting contribution were to overwhelm the contribution from the normal grand potential deep enough into the superconducting state. Based on an approximate evaluation of the Gor'kov expansion parameters one can calculate an expression for H_{inv} .¹⁸ Using our expressions for the damping, we are able to predict that within the region of validity of the perturbative scheme this effect will not occur. Hence there is no theoretical reason, within perturbation theory, to expect inversion of the magnetic oscillations. This result agrees with the lack of experimental observation of such an effect. It also agrees with our exact numerical solutions to the BdG equations which show a complete suppression of the magnetic oscillations deep enough into the mixed state.²³

Although there are currently experimental uncertainties about the value of H_{c2} in the organic superconductors, a comparison with experimental results for the quasi-2D superconductor $\kappa\text{-(ET)}_2\text{Cu(NCS)}_2$ yields good agreement between theory and experiment.

The outline of our paper is as follows. Section II sets up the formalism for describing the vortex state using both the Bogoliubov–de Gennes equations and perturbation theory. In Sec. III we compare the results of the perturbation theory with the exact numerical solution. The damping of the magnetic oscillations is discussed in Sec. IV. We give a physical interpretation of the damping. The effect of a finite Zeeman splitting term is discussed and the case of a conserved number of particles as opposed to a conserved chemical potential is considered. Using approximate expressions for the damping parameters we are able to give a simple analytical expression for the rate of damping of the dHvA oscillations close to H_{c2} . The spin dependence and the temperature dependence of the oscillations can then be extracted. We then examine the validity of the arguments leading to a sign change of the first harmonic of the dHvA oscillations. In Sec. VI we compare our analytical theory with experimental results. Finally we summarize our results in Sec. VII.

II. ELECTRONS IN THE VORTEX STATE

A. General representation and BdG equations

We consider a pure 2D electron gas in the x - y plane with a perpendicular magnetic field H along the z axis. In the Landau gauge $\mathbf{A}=(0,Hx,0)$, the single-particle eigenstates can be chosen to be

$$\phi_{N,k}(\mathbf{r}) = \frac{1}{\sqrt{L_y}} e^{-iky} \phi_N\left(\frac{x-kl^2}{l}\right), \quad (1)$$

where $\phi_N(x) = (2^N N! \sqrt{\pi} l)^{-1/2} H_N(x) e^{-x^2/2}$, with H_N being a Hermite polynomial of order N , and $l^2 = \hbar c/eH$ is the magnetic length. The size of the system is $L_x \times L_y$. Band structure effects are assumed to be adequately described employing an electron effective mass m^* . The B field is taken to be uniform within the sample, thereby ignoring the partial screening by the supercurrents. This approximation holds for strong type-II superconductors ($\kappa \gg 1$) such as the organics, where the penetration depth is much larger than the coherence length.

In the mixed state of a conventional type-II superconductor the order parameter forms a vortex lattice. It is therefore advantageous to use a basis set which incorporates this symmetry. We have chosen to use the following set of functions introduced by Norman *et al.*¹⁷

$$\phi_{N\mathbf{k}}(\mathbf{r}) = \sqrt{\frac{a_x}{L_x}} \sum_t e^{ik_x a_x t} e^{i\pi t^2/4} \phi_{N, -k_y + t a_x/l^2}(\mathbf{r}), \quad (2)$$

where $k_x \in [0, 2\pi/a_x[$ with $\Delta k_x = 2\pi/L_x$ and $k_y \in [0, a_x/l^2[$ with $\Delta k_y = 2\pi/L_y$ define the magnetic Brillouin zone (MBZ). The symmetry of the order parameter restricts the pairing to be between electrons with quantum numbers \mathbf{k} and $-\mathbf{k}$.¹³ By adjusting a_x we can obtain both a triangular [$a_x = l(\sqrt{3}\pi/2)^{1/2}$] and a square vortex lattice [$a_x = l(\pi/2)^{1/2}$]. Throughout this paper we choose to work with the triangular lattice since we expect the free energy to be minimized by this symmetry (except possibly in the reentrant regime).¹⁷ We are using mean-field BCS theory with a smooth cutoff in the interaction around the Fermi surface, applicable for weak-coupling superconductors. The mean-field Hamiltonian is

$$\hat{H} = \hat{H}_0 + \hat{H}_1,$$

$$\hat{H}_0 = \int d\mathbf{r} \psi_\sigma^\dagger(\mathbf{r}) \left(\frac{[\mathbf{p} - (e/c)\mathbf{A}]^2}{2m} - \mu \right) \psi_\sigma(\mathbf{r}),$$

$$\begin{aligned} \hat{H}_1 = & \sum_{\substack{NM \\ \mathbf{k}}} \int d\mathbf{r} [\Delta(\mathbf{r}) w(N) w(M) \\ & \times \phi_{M\mathbf{k}}^*(\mathbf{r}) \phi_{N-\mathbf{k}}^*(\mathbf{r}) \hat{a}_{M\mathbf{k}\uparrow}^\dagger \hat{a}_{N-\mathbf{k}\downarrow}^\dagger + \text{c.c.}], \end{aligned} \quad (3)$$

where the order parameter is defined as

$$\Delta(\mathbf{r}) \equiv V \sum_{\substack{NM \\ \mathbf{k}}} w(N) w(M) \phi_{N\mathbf{k}}(\mathbf{r}) \phi_{M-\mathbf{k}}(\mathbf{r}) \langle a_{N\mathbf{k}\uparrow} a_{M-\mathbf{k}\downarrow} \rangle \quad (4)$$

This differs from the conventional BCS Hamiltonian since we have introduced the weight function $w(n)$. It is necessary to have a smooth cutoff in the pairing interaction since we otherwise would get nonphysical effects arising from Landau levels abruptly entering or leaving the pairing region. The weight function $w(n)$ is chosen to be Gaussian, i.e., $w(N) \propto e^{-(\xi_N/0.5\hbar\omega_D)^2}$, where ω_D is the pairing width and $\xi_N = (N+1/2)\hbar\omega_c - \mu$. This approach was introduced by Norman *et al.*¹⁷ although they used a different weighting function. It should be noted that the above slightly unconventional definition of the order parameter is necessary. Otherwise the self-consistency condition is not equivalent to minimizing the grand potential Ω with respect to $\Delta(\mathbf{r})$ [i.e., $\delta\Omega/\delta\Delta(\mathbf{r})=0$]. In the vortex lattice case the order parameter can be characterized by a finite number of parameters Δ_j ,¹⁷

$$\Delta(\mathbf{r}) = \frac{V a_x}{\sqrt{L_y L_x}} \sum_j \Delta_j \sum_g e^{i\pi g^2/2} \phi_{j, \sqrt{2}g a_x}(\sqrt{2}\mathbf{r}). \quad (5)$$

The Δ_j 's are determined self-consistently as explained in Ref. 17. Assuming not only translational but also sixfold rotational symmetry of $|\Delta(\mathbf{r})|$ gives the restriction¹⁴ $j=0,6,12, \dots$, where $j \leq 2N_{\max} \cdot N_{\max}$ is the highest Landau level participating in the pairing. Using the above transformation the corresponding BdG equations split into a set of equations for each \mathbf{k} and they can be solved numerically. Norman *et al.*¹⁷ have carried out an extensive numerical investigation of the quasiparticle spectrum and the magnetic oscillations in the superconducting state. We have developed a similar numerical scheme to solve the BdG equations. In this way we are able to check our analytical results against an exact numerical solution.

B. Perturbative expansion of the grand potential

Since we are interested in the region near H_{c2} where the order parameter is small, it is natural to consider the Gor'kov expansion of the grand potential. This can be done either through the equation of motion approach originally used or by using the grand partition function for the symmetry-broken self-consistent Hamiltonian:

$$\mathcal{Z} = \int \mathcal{D}(\psi_\sigma^*(\mathbf{r}, \tau) \psi_\sigma(\mathbf{r}, \tau)) \exp\left(-\int_0^\beta d\tau \int d\mathbf{r} \mathcal{L}(\mathbf{r}, \tau)\right),$$

$$\begin{aligned} \mathcal{L}(\mathbf{r}, \tau) = & \psi_\sigma^*(\mathbf{r}, \tau) \left(\partial_\tau + \frac{[\mathbf{p} - (e/c)\mathbf{A}]^2}{2m} - \mu \right) \psi_\sigma(\mathbf{r}, \tau) \\ & - \left[\Delta(\mathbf{r}) \tilde{\psi}_\uparrow^*(\mathbf{r}, \tau) \tilde{\psi}_\uparrow^*(\mathbf{r}, \tau) + \text{c.c.} - \frac{1}{V} |\Delta(\mathbf{r})|^2 \right], \end{aligned} \quad (6)$$

where $\mathcal{D}(\psi_\sigma^*(\mathbf{r}, \tau) \psi_\sigma(\mathbf{r}, \tau))$ denotes functional integration over Grassman variables. We have defined $\tilde{\psi}_\sigma(\mathbf{r}) = \sum_{n, \mathbf{k}} w(n) \phi_{n, \mathbf{k}}(\mathbf{r}) a_{n, b f k \sigma}$. The $(1/V)|\Delta(\mathbf{r})|^2$ term corrects for the double counting of the interaction energy in the Hartree-Fock approximation. Expanding the grand potential $\Omega = (-1/\beta) \ln \mathcal{Z}$ in powers of $\Delta(\mathbf{r})$ we obtain to eighth order

$$\Omega_S - \Omega_N = \Omega_2 + \Omega_4 + \Omega_6 + \Omega_8, \quad (7)$$

where

$$\begin{aligned} \Omega_2 &= \frac{1}{V} \int d\mathbf{r} |\Delta(\mathbf{r})|^2 - \frac{1}{\beta} \int d\mathbf{r}_1 d\mathbf{r}_2 \Delta(\mathbf{r}_1) \Delta^*(\mathbf{r}_2) K_2(\mathbf{r}_1, \mathbf{r}_2), \\ \Omega_4 &= \frac{1}{2\beta} \int d\mathbf{r}_1 \cdots d\mathbf{r}_4 K_4(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) \Delta(\mathbf{r}_1) \Delta(\mathbf{r}_2) \Delta^*(\mathbf{r}_3) \Delta^*(\mathbf{r}_4), \\ \Omega_6 &= -\frac{1}{3\beta} \int d\mathbf{r}_1 \cdots d\mathbf{r}_6 K_6(\mathbf{r}_1, \dots, \mathbf{r}_6) \Delta(\mathbf{r}_1) \Delta(\mathbf{r}_2) \Delta(\mathbf{r}_3) \Delta^*(\mathbf{r}_4) \Delta^*(\mathbf{r}_5) \Delta^*(\mathbf{r}_6), \\ \Omega_8 &= \frac{1}{4\beta} \int d\mathbf{r}_1 \cdots d\mathbf{r}_8 K_8(\mathbf{r}_1, \dots, \mathbf{r}_8) \Delta(\mathbf{r}_1) \Delta(\mathbf{r}_2) \Delta(\mathbf{r}_3) \Delta(\mathbf{r}_4) \Delta^*(\mathbf{r}_5) \Delta^*(\mathbf{r}_6) \Delta^*(\mathbf{r}_7) \Delta^*(\mathbf{r}_8). \end{aligned} \quad (8)$$

The kernels are given by

$$\begin{aligned} K_2(\mathbf{r}_1, \mathbf{r}_2) &= \frac{1}{\hbar^2} \sum_\nu \tilde{G}_\uparrow^0(\mathbf{r}_2, \mathbf{r}_1, -\omega_\nu) \tilde{G}_\downarrow^0(\mathbf{r}_2, \mathbf{r}_1, \omega_\nu), \\ K_4(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) &= \frac{1}{\hbar^4} \sum_\nu \tilde{G}_\downarrow^0(\mathbf{r}_4, \mathbf{r}_1, \omega_\nu) \tilde{G}_\uparrow^0(\mathbf{r}_3, \mathbf{r}_1, -\omega_\nu) \tilde{G}_\downarrow^0(\mathbf{r}_3, \mathbf{r}_2, \omega_\nu) \tilde{G}_\uparrow^0(\mathbf{r}_4, \mathbf{r}_2, -\omega_\nu), \\ K_6(\mathbf{r}_1, \dots, \mathbf{r}_6) &= \frac{1}{\hbar^6} \sum_\nu \tilde{G}_\downarrow^0(\mathbf{r}_6, \mathbf{r}_1, \omega_\nu) \tilde{G}_\uparrow^0(\mathbf{r}_5, \mathbf{r}_1, -\omega_\nu) \tilde{G}_\downarrow^0(\mathbf{r}_5, \mathbf{r}_2, \omega_\nu) \tilde{G}_\uparrow^0(\mathbf{r}_4, \mathbf{r}_2, -\omega_\nu) \tilde{G}_\downarrow^0(\mathbf{r}_4, \mathbf{r}_3, \omega_\nu) \tilde{G}_\uparrow^0(\mathbf{r}_6, \mathbf{r}_3, -\omega_\nu), \\ K_8(\mathbf{r}_1, \dots, \mathbf{r}_8) &= \frac{1}{\hbar^8} \sum_\nu \tilde{G}_\downarrow^0(\mathbf{r}_6, \mathbf{r}_1, \omega_\nu) \tilde{G}_\uparrow^0(\mathbf{r}_7, \mathbf{r}_1, -\omega_\nu) \tilde{G}_\downarrow^0(\mathbf{r}_7, \mathbf{r}_2, \omega_\nu) \tilde{G}_\uparrow^0(\mathbf{r}_8, \mathbf{r}_2, -\omega_\nu) \tilde{G}_\downarrow^0(\mathbf{r}_5, \mathbf{r}_3, \omega_\nu) \\ &\quad \times \tilde{G}_\uparrow^0(\mathbf{r}_6, \mathbf{r}_3, -\omega_\nu) \tilde{G}_\downarrow^0(\mathbf{r}_8, \mathbf{r}_4, \omega_\nu) \tilde{G}_\uparrow^0(\mathbf{r}_5, \mathbf{r}_4, -\omega_\nu), \end{aligned} \quad (9)$$

and $\omega_\nu = (2\nu + 1)\pi k_B T / \hbar$ are the Matsubara frequencies. Maniv *et al.*¹⁹ have calculated the expansion up to fourth order in $\Delta(\mathbf{r})$ using essentially semiclassical approximations. They used a variational form of the order parameter which has no symmetry built in initially but restricts the electrons to condense in the lowest center-of-mass Landau level ($\Delta_{j \neq 0} = 0$). As will be shown below, this restriction introduces no serious error within in the region of interest in the phase diagram. Since it is known¹⁷ that the triangular lattice is the minimal energy configuration (except for the reentrant regime), we have exploited this symmetry to calculate these expansion terms exactly. Because we are using a smooth pairing cutoff in our Hamiltonian we have, instead of the Green's function for the normal state $G_\sigma^0(\mathbf{r}_2, \mathbf{r}_1, \omega_\nu)$, the following function in our kernels:

$$\tilde{G}_\sigma^0(\mathbf{r}_2, \mathbf{r}_1, \omega_\nu) = \sum_{n\mathbf{k}} \frac{\phi_{n\mathbf{k}}(\mathbf{r}_2) \phi_{n\mathbf{k}}^*(\mathbf{r}_1)}{i\omega_\nu - \xi_{n\sigma}/\hbar} w^2(n), \quad (10)$$

where $\xi_{n\sigma} = \xi_n + gm^* \sigma / 2m_0 \hbar \omega_c$. The only difference from the Green's function for the normal state is that we have included the weight functions $w(n)$ in the sum. Using the symmetry of the vortex lattice the integrals can be solved. We have to fourth order

$$\Omega_2 = \frac{Va_x}{\sqrt{2}lL_x L_y} \sum_j \left[1 - \frac{V}{4\pi l^2} \sum_{n_1, n_2} B_j^{n_1 n_2} w^2(n_1) w^2(n_2) \frac{\tanh(\beta \xi_{n_1 \downarrow} / 2) + \tanh(\beta \xi_{n_2 \uparrow} / 2)}{2(\xi_{n_1 \downarrow} + \xi_{n_2 \uparrow})} \right] \Delta_j^2 = \sum_j \alpha_j \Delta_j^2 \quad (11)$$

and

$$\begin{aligned}
\Omega_4 &= \frac{V^4 a_x^4}{8L_x^4 L_y^4 L_z^4} \sum_{n_1 \dots n_4} w^2(n_1) w^2(n_2) w^2(n_3) w^2(n_4) f(n_1, n_2, n_3, n_4) \\
&\quad \times \sum_{j_1 \dots j_4} B_{j_1}^{n_1 n_4} B_{j_2}^{n_3 n_2} B_{j_3}^{n_1 n_2} B_{j_4}^{n_3 n_4} \Xi_{n_1+n_4-j_1, n_2+n_3-j_2}^{n_1+n_4-j_1, n_2+n_3-j_2} \Delta_{j_1} \Delta_{j_2} \Delta_{j_3} \Delta_{j_4} \\
&= \sum_{j_1 \dots j_4} \gamma_{j_1 \dots j_4} \Delta_{j_1} \Delta_{j_2} \Delta_{j_3} \Delta_{j_4}, \tag{12}
\end{aligned}$$

where

$$f(n_1, n_2, n_3, n_4) = \frac{1}{\beta} \sum_{\nu} [(-i\hbar\omega_{\nu} - \xi_{n_1\downarrow})(i\hbar\omega_{\nu} - \xi_{n_2\uparrow})(-i\hbar\omega_{\nu} - \xi_{n_3\downarrow})(i\hbar\omega_{\nu} - \xi_{n_4\uparrow})]^{-1} \tag{13}$$

and

$$\begin{aligned}
\Xi_{j_3 j_4}^{j_1 j_2} &= \frac{L_x L_y}{4\pi a_x} \sum_j B_j^{j_1 j_2} B_j^{j_3 j_4} \sum_{h_1 h_2} e^{-i\pi(h_1^2 - h_2^2)} [\phi_{j_1+j_2-j}(2h_1 a_x) \phi_{j_3+j_4-j}(2h_2 a_x) \\
&\quad + e^{-i\pi(h_1 - h_2)} \phi_{j_1+j_2-j}(2h_1 a_x + a_x) \phi_{j_3+j_4-j}(2h_2 a_x + a_x)]. \tag{14}
\end{aligned}$$

The coefficient B_j^{NM} is defined as

$$B_j^{N,M} \equiv \left(\frac{j!(N+M-j)!N!M!}{2^{N+M}} \right)^{1/2} \sum_{m=\max(0, j-N)}^{\min(j, M)} \frac{(-1)^{M-m}}{(j-m)!(N+m-j)!(M-m)!m!}. \tag{15}$$

The sums over states above are restricted to Landau levels lying within the pairing width around the chemical potential. Using the standard method of evaluating Matsubara sums by contour integration we obtain

$$\begin{aligned}
f(n_1, n_2, n_3, n_4) &= [(e^{-\beta\xi_{n_1\downarrow}} + 1)(\xi_{n_1\downarrow} + \xi_{n_2\uparrow})(-\xi_{n_1\downarrow} + \xi_{n_3\downarrow})(\xi_{n_1\downarrow} + \xi_{n_4\uparrow})]^{-1} + [(e^{\beta\xi_{n_2\uparrow}} + 1)(\xi_{n_2\uparrow} + \xi_{n_1\downarrow})(\xi_{n_2\uparrow} + \xi_{n_3\downarrow}) \\
&\quad \times (\xi_{n_2\uparrow} - \xi_{n_4\uparrow})]^{-1} + [(e^{-\beta\xi_{n_3\downarrow}} + 1)(-\xi_{n_3\downarrow} + \xi_{n_1\downarrow})(\xi_{n_3\downarrow} + \xi_{n_2\uparrow})(\xi_{n_3\downarrow} + \xi_{n_4\uparrow})]^{-1} + [(e^{\beta\xi_{n_4\uparrow}} + 1)(\xi_{n_4\uparrow} + \xi_{n_1\downarrow}) \\
&\quad \times (\xi_{n_4\uparrow} - \xi_{n_2\uparrow})(\xi_{n_4\uparrow} + \xi_{n_3\downarrow})]^{-1}. \tag{16}
\end{aligned}$$

The second-order term Ω_2 which determines the H_{c2} line agrees, apart from the inclusion of the weight function, with the result of MacDonald *et al.*²⁴ and Rajagopal and Ryan.²⁵ The sixth and eighth-order terms Ω_6 and Ω_8 can also be calculated and they are given in Appendix A. We get the form

$$\begin{aligned}
\Omega_S - \Omega_N &= \sum_j \alpha_j(T, H) \Delta_j^2 + \sum_{j_1 \dots j_4} \gamma_{j_1 \dots j_4}(T, H) \Delta_{j_1} \dots \Delta_{j_4} + \sum_{j_1 \dots j_6} \kappa_{j_1 \dots j_6}(T, H) \Delta_{j_1} \dots \Delta_{j_6} \\
&\quad + \sum_{j_1 \dots j_8} \eta_{j_1 \dots j_8}(T, H) \Delta_{j_1} \dots \Delta_{j_8}. \tag{17}
\end{aligned}$$

Thus we have derived the exact quantum-mechanical expressions for the expansion coefficients for $\Omega_S - \Omega_N$ up to eighth order assuming a vortex lattice. We have not yet restricted the electrons to form pairs with the lowest possible center-of-mass energy ($j=0$). The result is a multidimensional polynomial in Δ_j . Going to eighth order permits us to check the convergence properties of the series. We could in principle calculate the expansion coefficients to any order but, as usual, the algebra gets more cumbersome with increasing order, and the minimization condition cannot be solved analytically for such high orders.

C. Self-consistency and minimization of Ω_S

The self-consistent determination of $\Delta(\mathbf{r}) \equiv V \langle \psi_{\uparrow}(\mathbf{r}) \psi_{\downarrow}(\mathbf{r}) \rangle$ is equivalent to minimizing the grand po-

tential with respect to $\Delta(\mathbf{r})$.²⁶ In the above formulation, which takes into account the spatial symmetry of the order parameter, this reduces to minimizing our multidimensional polynomial with respect to Δ_j . Although this is a standard numerical problem it is necessary to make further approximations in order to obtain simple analytical results. The instability towards superconductivity is determined by the sign of the expansion coefficients α_j . Above H_{c2} we have $\alpha_j > 0$ for all j . The transition to the mixed vortex state occurs when one of the α_j 's becomes negative. The system can then lower its energy by making the corresponding Δ_j non-zero. It has been shown that the instability occurs first in the $j=0$ channel.²⁴ So we have $\alpha_0 < 0$ and $\alpha_{j \neq 0} > 0$ for $H \leq H_{c2}$ and therefore $\Delta_0 \gg \Delta_{j \neq 0}$. We can then make the approximation $\Delta_{j \neq 0} = 0$, i.e., only consider condensation

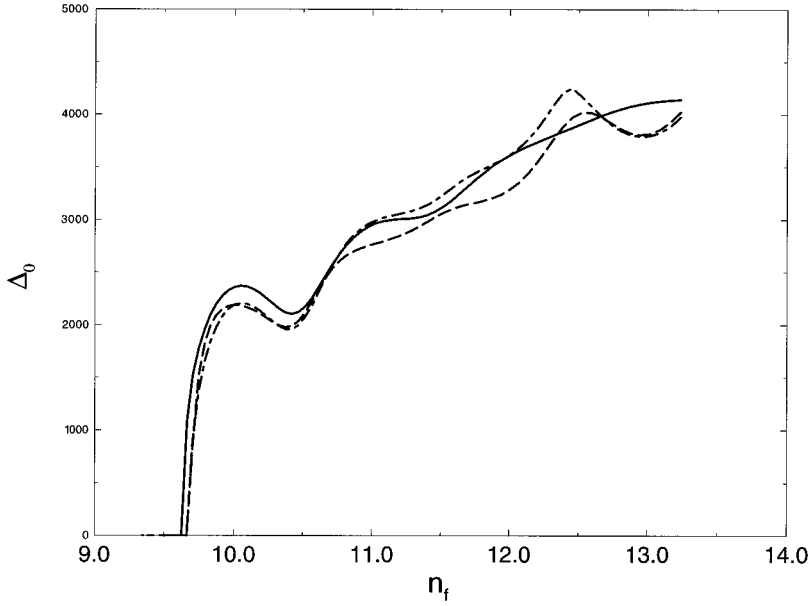


FIG. 1. The order parameter Δ_0 vs n_f calculated numerically (solid line), to fourth order in Δ_0 (dashed line), and to eighth order in Δ_0 (dash-dotted line).

into pairs with lowest Landau level center-of-mass motion. We have checked this approximation by solving the BdG equation numerically when $\Delta_{j \neq 0} = 0$ and when all the Δ_j 's are nonzero. In the region of interest there is essentially no difference between the two solutions thus justifying our approximation.

The grand potential now has the Landau form

$$\alpha \Delta_0^2 + \gamma \Delta_0^4 + \kappa \Delta_0^6 + \eta \Delta_0^8 \quad (18)$$

($\alpha = \alpha_0$, $\gamma = \gamma_{0000}$, etc.), and our self-consistency problem is reduced to a simple one-dimensional minimization problem which can be easily solved. To fourth order we have a Mexican hat potential when we are in the mixed state ($\alpha < 0$ and $\gamma > 0$) and the minimum for the grand potential is obtained for nonzero Δ_0 . Requiring $\partial_{\Delta_0}(\Omega_S - \Omega_N)|_{\tilde{\Delta}_0} = 0$ gives

$$z^3 + a_1(T, H)z^2 + a_2(T, H)z + a_3(T, H) = 0, \quad (19)$$

where $z = \tilde{\Delta}_0^2$ and $a_1 = 3\kappa/4\eta$, $a_2 = \gamma/2\eta$, and $a_3 = \alpha/4\eta$. $\tilde{\Delta}_0$ is the value of Δ_0 which minimizes $\Omega_S - \Omega_N$. Equation (19) is a cubic equation and can be solved exactly. To fourth order we obtain

$$\tilde{\Delta}_0^2 = -\frac{\alpha(T, H)}{2\gamma(T, H)}, \quad \Omega_S - \Omega_N = -\frac{\alpha^2(T, H)}{4\gamma(T, H)}. \quad (20)$$

Equation (19) yields $\tilde{\Delta}_0$ and therefore $\Delta(\mathbf{r})$ and $\Omega_S - \Omega_N$ as a function of H . The value $\tilde{\Delta}_0$ which minimizes $\Omega_S - \Omega_N$ will be a function of H and T through the coefficients $\alpha, \gamma, \kappa, \eta$. Because magnetic quantization has been accounted for exactly, all coefficients and, hence, $\tilde{\Delta}_0$ and $\Omega_S - \Omega_N$ are oscillating functions of H for a given temperature T . The condensation energy $\Omega_S - \Omega_N$ oscillates 180° out of phase with the normal state Ω_N close to H_{c2} . This is the origin of the damping of the magnetic oscillations of Ω_S compared to Ω_N . The physical reason for this effect is rather simple as will be explained in Sec. IV A.

We now consider the magnetization $M_S \equiv (\partial_H \Omega_S)_\mu = (\partial_H(\Omega_N + [\Omega_S - \Omega_N]))_\mu$. The grand potential for a free 2D electron gas Ω_N can be calculated analytically for the case when only two Landau levels are partially occupied.^{27,28} For relatively high T , low H , or small g factor, this assumption breaks down, but it is then straightforward to calculate Ω_N numerically. It should be noted that the chemical potential μ in general is a function of H . We have in most of this article, for simplicity, kept the chemical potential μ fixed thereby avoiding having to determine μ self-consistently. The oscillatory effect of the chemical potential is most important for low temperatures ($T \leq 0.2$) and very clean samples such that higher harmonics contribute to the magnetic oscillations. In Sec. IV C we will show that even in this case one can to a good approximation consider the chemical potential constant in the mixed state.

III. COMPARISON BETWEEN NUMERICAL DATA AND PERTURBATION EXPANSION

Recently it has been claimed that the degeneracy of the Landau levels should give rise to nonperturbative terms in the expression for $\Omega_S - \Omega_N$ making the Gor'kov theory invalid. For finite temperature there should be a non-perturbative Δ_0^3 term in Eq. (18) resulting in many interesting thermodynamic effects.²¹ It is therefore of importance to establish the validity of the perturbation theory developed in the preceding sections so that we can use it to derive results instead of a cumbersome numerical solution. This is essential in the case when many Landau levels participate in the pairing since the computation time is very long in this regime for the numerical solution. In order to estimate the accuracy of our perturbation expansion, we compare it to an exact numerical solution of the corresponding BdG equations. As mentioned earlier, we have set up a code which solves these equations self-consistently. We have chosen parameters such that $\omega_D/\omega_c = 5$, $V/\hbar\omega_c l^2 = 8.2$, and $k_B T/\hbar\omega_c = 0.28$ when $n_f = 12$. In Fig. 1 we show the order parameter $\tilde{\Delta}_0$ as a function of the magnetic field. The chemical potential μ is fixed. We have plotted the numerical, fourth-order, and eighth-order solutions. There is good agreement between the numerical solution and our perturbation expansion for both

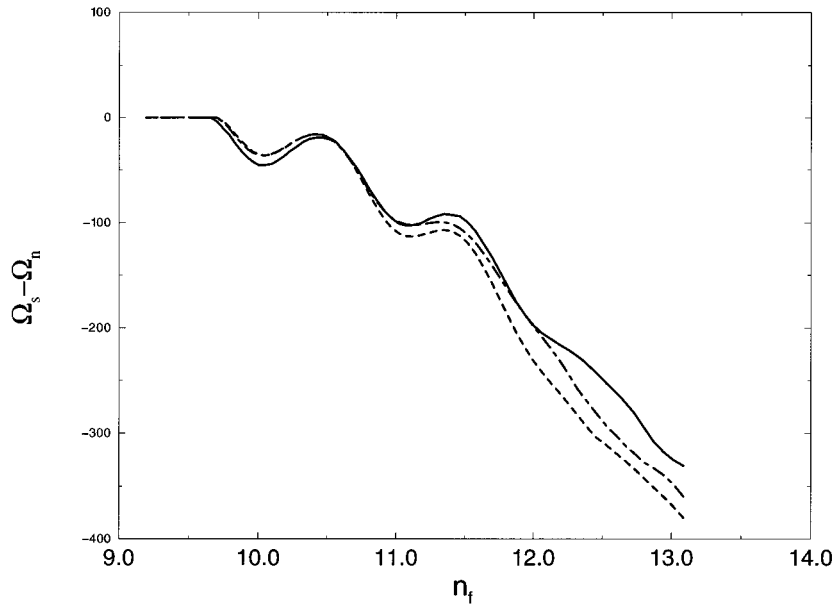


FIG. 2. The difference $\Omega_S - \Omega_N$ in the grand potential between the mixed state and the normal state. The solid line is a numerical calculation, the dashed line is fourth-order perturbation theory, and the dash-dotted line is eighth-order perturbation theory.

fourth and eighth order. The general behavior of Δ_0 is correctly predicted by both the fourth- and eighth-order expansions. In Fig. 2 we have plotted the condensation energy $\Omega_S - \Omega_N$. We are measuring energies in units of $\hbar\omega_c$. It is apparent that the contribution $\Omega_S - \Omega_N$ has local minima for n_f integer. Since Ω_N has local maxima for n_f integer, the condensation energy oscillates 180° out of phase with the contribution from the normal-state Ω_N . We therefore get partial cancellation of the normal-state oscillations and a damping of the dHvA oscillations. This is seen in Fig. 3 where we have plotted the magnetization $M \equiv -(\partial_H \Omega)_\mu$ for both the normal state and the mixed state. When the superconducting order starts to increase at $n_f \approx 10$, we get significant damping of the dHvA oscillations. Again the agreement with the numerical data is good as long as $n_f \lesssim 12$. Eighth-order theory tends to agree better with numerical data than does the fourth-order theory, indicating that the perturbation expansion is valid. Once we go too far into the superconducting state, the perturbation theory starts to disagree with

the numerical results, also as expected. We see from Fig. 1 and Fig. 2 that the magnitude of Δ_0 and $\Omega_S - \Omega_N$ is still fairly well described for $n_f > 12$, but both fourth- and eighth-order expansions start to pick up spurious oscillations in the order parameter and in the energy. $\Omega_S - \Omega_N$ actually starts to oscillate in phase with Ω_N according to the perturbation theory. This gives enhancement of the dHvA oscillations in the mixed state as compared to the normal state, as seen from Fig. 3. This is an unphysical effect and is absent in the exact solution. Since this enhancement is neither confirmed numerically nor experimentally, we conclude that perturbation theory in the single parameter Δ_0 breaks down at this point. It can be shown²² that the Gor'kov expansion is convergent if the change in the quasiparticle energies $|E_{\mathbf{k}}^\eta - \xi_\eta|$ is not larger than $O(k_B T)$. We have looked at the numerically calculated quasiparticle energies as a function of n_f . As expected and in agreement with Norman *et al.*¹⁷ we observe that the quasiparticle bands go from being essentially broadened Landau levels close to the transition point to losing all

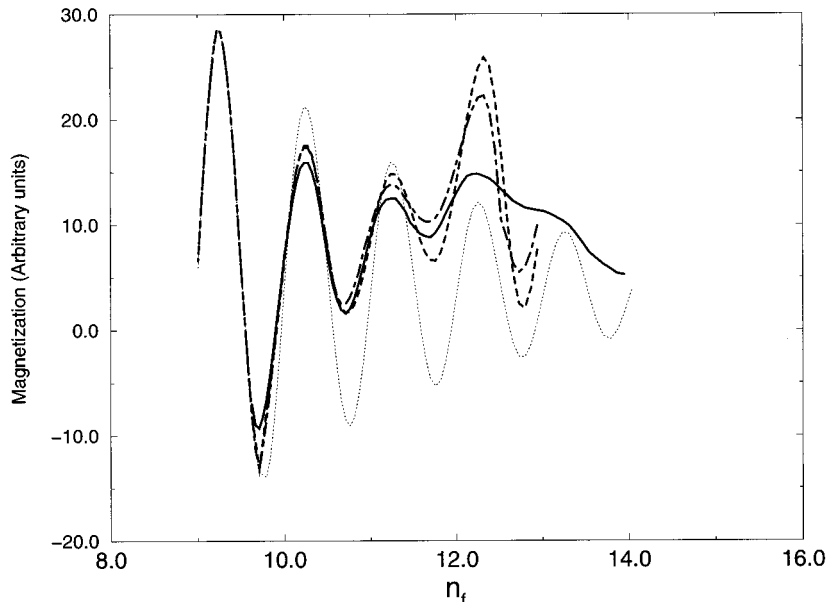


FIG. 3. The magnetization vs n_f . The solid line is a numerical calculation, the dashed line fourth order, the dash-dotted line eighth order, and the dotted line is the magnetization in the underlying normal state.

their Landau level structure deeper into the mixed state. For the above specific case we have found that for $n_f \gtrsim 12$ the quasiparticle energies are changed so much that the above condition for the validity of the Gor'kov series does not hold in large regions of \mathbf{k} space, thus explaining the breakdown of perturbation theory. We have compared the numerical solution and the perturbation expansion for a number of different parameters. Our conclusion is that both fourth- and eighth-order perturbation theories describe well the superconducting state and the corresponding damping of the magnetic oscillations near the transition point. However, the perturbation theory eventually breaks down when the quasiparticle levels are changed too much, in the sense described above. The convergence range of the Gor'kov expansion is determined by the temperature $k_B T$.

The numerical results show total suppression of the dHvA effect once we are deep enough into the mixed state. In Fig. 3 the numerical solution shows that M_s loses its dHvA structure completely for $n_f \gtrsim 12$. This contradicts the recent predictions of a sign shift of the first harmonic of the dHvA oscillations.¹⁸ This prediction is partly based on the assumption that the quasiparticle spectrum can be described by a simple splitting of the Landau levels into two levels symmetrically placed on around each Landau level even when the actual change in energy is rather large ($|E_{\mathbf{k}}^\eta - \xi_\eta|/\hbar\omega_c \approx \pm 0.22$). We have found that the low-lying quasiparticle levels lose their Landau level structure and describe essentially localized bound states when the change in energies is of the above magnitude. This crossover to localized states makes the argument leading to the sign change of the first harmonic invalid and it leads to the suppression of the magnetic oscillations.²³

IV. DAMPING OF THE MAGNETIC OSCILLATIONS

A. Physical interpretation

To get a physical understanding of the superconducting damping of the magnetic oscillations, it is helpful to consider the ground state which gives the dominant contribution to the ground potential for low temperatures. By analogy with the case of no magnetic field,²⁹ our numerical solution is based on the following canonical transformation:

$$\hat{\gamma}_{\mathbf{k}\uparrow}^\eta = \sum_N [u_{N\mathbf{k}}^{*\eta} \hat{a}_{N\mathbf{k}\uparrow} + v_{N\mathbf{k}}^{*\eta} \hat{a}_{N-\mathbf{k}\downarrow}^\dagger], \quad (21)$$

$$\hat{\gamma}_{\mathbf{k}\downarrow}^\eta = \sum_N [u_{N\mathbf{k}}^{*\eta} \hat{a}_{N\mathbf{k}\downarrow} - v_{N\mathbf{k}}^{*\eta} \hat{a}_{N-\mathbf{k}\uparrow}^\dagger], \quad (22)$$

where $u_{N\mathbf{k}}^\eta$ is the coefficient of $\phi(\mathbf{r})_{N\mathbf{k}}$ and $v_{N\mathbf{k}}^\eta$ is the coefficient of $\phi^*(\mathbf{r})_{N-\mathbf{k}}$ in the Bogoliubov amplitudes $u(\mathbf{r})$ and $v(\mathbf{r})$ for the η th solution, respectively. The corresponding ground state of our mean-field Hamiltonian is then

$$|\Psi_g\rangle \propto \prod_{\eta\mathbf{k}} \hat{\gamma}_{\mathbf{k}\uparrow}^\eta \hat{\gamma}_{-\mathbf{k}\downarrow}^\eta |\Psi\rangle, \quad (23)$$

where $|\Psi\rangle$ is a state with all single-particle states with energy less than $\mu - \omega_D$ empty and all single-particle states with energy higher than $\mu + \omega_D$ occupied. We see that Eq. (23) gives a coherent superposition of states where the pairs

$\hat{a}_{N\mathbf{k}}^\dagger \hat{a}_{N'-\mathbf{k}}^\dagger |0\rangle$ are either occupied or unoccupied. When we have a Landau level at the chemical potential μ ($n_f = \text{integer}$) it does not cost any kinetic energy to make a superposition of states with either occupied or unoccupied pairs formed by electrons in that level. The instability towards superconductivity is therefore largest when we have $\mu = (n + 1/2)\hbar\omega$. Since the grand potential of the normal state is at a maximum³⁰ when $\mu = (n + 1/2)\hbar\omega$, we have that $\Omega_S - \Omega_N$ and Ω_N oscillate 180° out of phase. This analysis is true for both constant chemical potential and constant number of particles. In the latter case one works with the Helmholtz free energy but the conclusions are the same. Mathematically the maximum in the damping comes from the fact that when the chemical potential is at a Landau level the sum in Eq. (11) is dominated by the terms with zero denominators, as an application of l' Hopital's rule on these terms confirms. Hence $\alpha(H)$ has a local minimum and the superconducting order a local maximum. This is the physical picture of the damping of the magnetic oscillations that naturally emerges from our formalism.

Norman *et al.*¹⁷ interpret the damping of the magnetic oscillations as an effect of the broadening of the Landau levels (LL's) due to superconducting order. An alternate explanation has been put forward Miller and Györfy,¹⁶ that emphasizes the role of nondiagonal pairing. There is in fact an intimate link between the two approaches that we now elucidate by the following simple calculation: We estimate $\Omega_S - \Omega_N$ (for simplicity we consider $T=0$) for the two cases when (I) the chemical potential is at a Landau level (n_f integer, maximum of the free energy) and (II) when it is exactly between two LL (n_f is half an odd integer, minimum of the free energy). In both cases we diagonalize the BdG equations approximately, but insist on using degenerate perturbation theory, because the diagonal approximation breaks down. When n_f is an integer, perturbation theory yields for the quasiparticle energy $E_{n_f\mathbf{k}} = |F_{n_f\mathbf{k}}|$. It can easily be seen that the contributions of the other LL to the ground-state energy cancel pairwise within degenerate perturbation theory (essentially because within degenerate perturbation theory level repulsion is symmetric with respect to the unperturbed degenerate level). Therefore the reduction in the maximum of the free energy for case (I) in the mixed state is

$$\Omega_S^I - \Omega_N^I \sim -\frac{1}{2} \sum_{\mathbf{k}} |F_{n_f\mathbf{k}}|$$

to lowest order in the pairing self-energy.

A similar calculation for case (II), when n_f is half an odd integer and the free energy is a minimum, gives an energy shift which is of higher than linear order in the pairing self-energy, because degenerate perturbation theory now leads to complete pairwise canceling for all Landau levels to first order in the pairing self-energy. Therefore the minimum of the oscillation is reduced by substantially less than the maximum, which shows that the damping of the oscillations is a direct consequence of the broadening of the quasiparticle levels accompanied by the mixed orbital character of quasiparticle excitations.

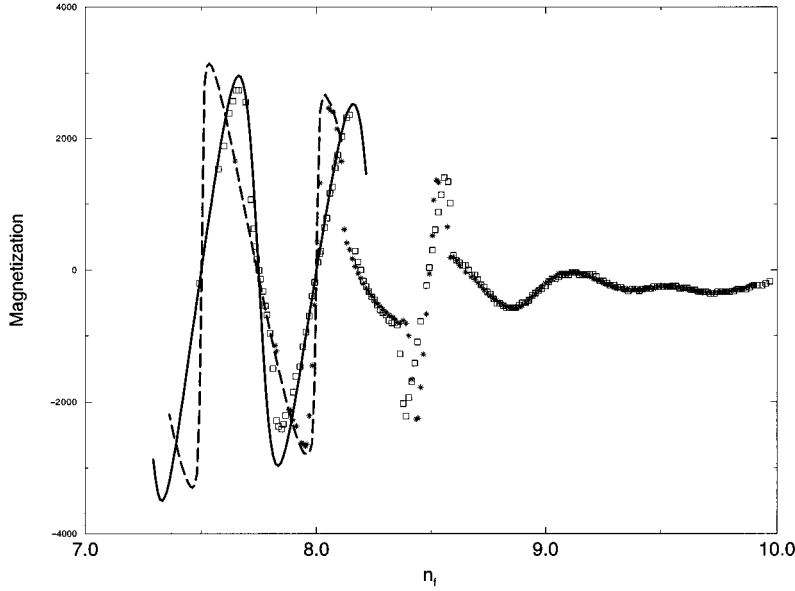


FIG. 4. The magnetization when the chemical potential is constant (\square) and when the number of particles is constant ($*$) for a very low temperature. The solid and dashed lines are the normal-state magnetization for fixed chemical potential and fixed number of particles, respectively.

B. Finite Zeeman splitting

Inclusion of spin in general reduces the magnitude of oscillations of Δ_0 and $\Omega_S - \Omega_N$. This reduction in the amplitude of the oscillations is due to the fact that spin-up and spin-down electrons now have different energy (unless $g = 2nm_0/m^*$, $n=0,1,2, \dots$). We can never have the situation whereby pairing occurs without a cost in kinetic energy. The oscillatory effect is therefore damped. The mathematical reason for the reduction in oscillations is that for finite spin the numerator in Eq. (11) never becomes zero. So we expect the magnetic oscillations in the mixed state to be reduced due to spin. The question is whether this reduction is larger or smaller than the corresponding reduction in the normal state, thus giving rise to extra damping effects. For temperatures (or impurity concentrations) such that only the first harmonic of the dHvA oscillations is important in both the mixed and the normal state ($k_B T \gtrsim 0.2\hbar\omega_c$) and within the region of validity of the perturbation expansion of $\Omega_S - \Omega_N$ the result is that the amplitude of the first harmonic of the dHvA oscillations in the mixed state is reduced by a factor $\cos(\pi gm^*/2m_0)$. This is the same reduction as in the normal state and hence the relative damping due to superconductivity is insensitive to spin splitting. This result will be proved in Sec. V. We have confirmed this result by solving the BdG equations numerically with and without a finite Zeeman splitting. The reduction in the amplitude in both the mixed and in the normal state as compared to the amplitude with no spin splitting corresponds very well to a $\cos(\pi gm^*/2m_0)$ factor in the region where the mixed state is described well by the perturbation expansion. Deeper into the mixed state the numerical results indicate that the effect of spin is suppressed by the superconducting order. The reduction in the amplitude of the magnetic oscillations due to a finite Zeeman term is less than the $\cos(\pi gm^*/2m_0)$ factor. This is due to the fact that when the superconducting order increases, the pairing interaction starts to dominate the Zeeman term and the effect of any finite g factor is suppressed.

So we conclude that within the region described well by our perturbative expansion a finite Zeeman term does not alter the rate of the damping of the magnetic oscillations due

to superconductivity. When only the first harmonic is important the effect of the Zeeman term is simply a reduction by a factor $\cos(\pi gm^*/2m_0)$ for the amplitude of the oscillations in both the mixed and in the normal state. Deeper into the mixed state the superconducting order starts to suppress the effect of the spin splitting and the magnetic oscillations is less affected by a finite Zeeman term. Hence in this region the relative size of the magnetic oscillations in the mixed state as compared to the normal state is larger for finite spin splitting and the damping is less efficient as compared to the $g=0$ case.

C. Conserved number of particles

For two-dimensional systems with a fixed number of particles it is well known³⁰ that the magnetic field dependence of the chemical potential $\mu(H)$ has a strong effect on the magnetic oscillations in a normal metal when higher harmonics are important. For low temperatures and clean samples the shape of the oscillations look qualitatively different when the chemical potential is fixed as compared to when the number of particles is fixed. We have up until now mainly considered the case of a constant chemical potential. When the number of particles is held fixed we need to consider Helmholtz free energy $F = \Omega + N\mu$. The chemical potential is determined by the equation

$$\langle \hat{N} \rangle = \sum_{\sigma \mathbf{N} \mathbf{k} \eta} [|u_{\mathbf{N} \mathbf{k}}^\eta|^2 f_{\sigma \mathbf{k}}^\eta + |v_{\mathbf{N} \mathbf{k}}^\eta|^2 (1 - f_{-\sigma \mathbf{k}})] = N \quad (24)$$

where $f_{\sigma \mathbf{k}}^\eta = [\exp(\beta E_{\sigma \mathbf{k}}^\eta) + 1]^{-1}$. This is a numerically cumbersome problem since we need to solve the BdG equations self-consistently for a given chemical potential, then calculate $\langle \hat{N} \rangle$, and repeat the calculation for a new value of μ until Eq. (24) is obeyed. However, it is essential that we determine the chemical potential self-consistently. If we naively assume that the chemical potential oscillates as in the normal state we would obtain persistent magnetic oscillations of the free energy even when the Landau level structure is completely destroyed by superconducting order. In Fig. 4

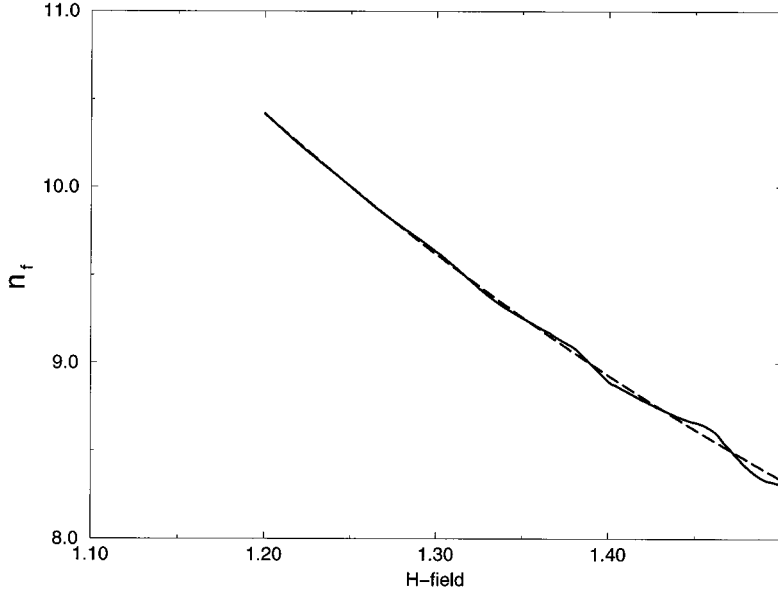


FIG. 5. n_f as a function of the magnetic field for fixed chemical potential (dashed line) and fixed number of particles (solid line).

we have plotted the magnetization when the chemical potential is constant (\square) and when the number of particles is constant ($*$) for a very low temperature. We have chosen parameters such that $\omega_D/\omega_c=5$, $V/\hbar\omega_c l^2=9.0$, $k_B T/\hbar\omega_c=0.05$, and $gm^*/m_0=1$ when $n_f=12$. For comparison the solid and dotted lines give the magnetization in the normal state for $n_f \gtrsim 8.2$ for conserved μ and N , respectively. We see that there is only a significant difference between the two curves close to H_{c2} ($n_f \approx 7.7$ at H_{c2}) when the chemical potential behaves differently in the two cases. Deeper into the mixed state the oscillatory behavior of the chemical potential is damped by the superconducting order and it becomes practically constant. This is illustrated in Fig. 5 where we have plotted $n_f = \mu(H)/\hbar\omega_c - 0.5$ as a function of the magnetic field ($H_{c2} \approx 1.5$) when the number of particles, N , is constant (solid line) and when the chemical potential is constant (dashed line). We see that the oscillations in the chemical potential when N is constant are damped in the mixed state. Once the superconducting order has damped the oscillations in the magnetization it has also damped the oscillation in $\mu(H)$ and the behavior for fixed N is essentially the same as for fixed μ . Thus the conclusion is that although there is some difference in the dHvA signal close to H_{c2} when N is fixed conserved as opposed to fixed μ the overall rate of damping of the oscillations is the same in the two cases.

V. SIMPLIFIED FORM FOR THE DAMPING

A. First harmonic of the condensation energy

To obtain a simple form for the damping, we must take a closer look at the coefficients $\alpha(H)$ and $\gamma(H)$ given in Eq. (11) and Eq. (12). As mentioned already, the transition to the mixed state occurs when $\alpha(H)$ changes sign. The Gor'kov expansion is most relevant for temperatures such that only the lowest harmonics of the dHvA signal are significant. This allows us to focus only on the zeroth and first harmonics of the relevant quantities. Thus we take $\alpha(H)$ to have the form

$$\alpha(H) \approx a_1(1 - H_{c2}/H) + a_2 \cos(2\pi\mu/\hbar\omega_c), \quad (25)$$

where $a_1 > 0$ and $a_2 > 0$. The coefficients a_1 and a_2 will in general depend weakly on the magnetic field but we assume they are constant. This is reasonable since for $\mu/\hbar\omega_c \gg 1$ the rate of change of a_1 and a_2 is very slow as compared to the frequency $\mu mc/\hbar e$ of the oscillations. The essential physics comes from the sign change of $\alpha(H)$ and its oscillatory behavior, combined with the features of $\gamma(H)$ described below. For simplicity we confine ourselves to fourth-order perturbation theory. The fourth-order coefficient $\gamma(H)$ has the form

$$\gamma(H) \approx g_1 - g_2 \cos(2\pi\mu/\hbar\omega_c), \quad (26)$$

where $g_1 > 0$ and $g_2 > 0$. Again both g_1 and g_2 depend on the magnetic field but this dependence is weak as compared to the strong oscillatory behavior coming from the Landau level structure. Note that we have opposite signs for the first harmonics of $\alpha(H)$ and $\gamma(H)$. In Sec. VB we will extract estimates of a_2 and g_2 from Eq. (11) and Eq. (12) whereas the approximate expressions for a_1 and g_1 will be given in Appendix B. Using these approximate forms for $\alpha(H)$ and $\gamma(H)$ we get for the condensation energy

$$\begin{aligned} \Omega_S - \Omega_N &= -\frac{\alpha^2(T, H)}{4\gamma(T, H)} \\ &\approx -\frac{[a_1(1 - H_{c2}/H) + a_2 \cos(2\pi\mu/\hbar\omega_c)]^2}{4[g_1 - g_2 \cos(2\pi\mu/\hbar\omega_c)]}. \end{aligned} \quad (27)$$

Assuming that $g_2 \ll g_1$ we get the following approximate form for the first harmonic of $\Omega_S - \Omega_N$ to first order in g_2/g_1 :

$$\begin{aligned} (\Omega_S - \Omega_N)_1 &\approx \frac{1}{4} \left[\frac{2a_1 a_2}{g_1} (H_{c2}/H - 1) - \frac{g_2 a_1^2}{g_1^2} (H_{c2}/H - 1)^2 \right. \\ &\quad \left. - \frac{3g_2 a_2^2}{4g_1^2} \right] \cos(2\pi\mu/\hbar\omega_c), \end{aligned} \quad (28)$$

where $\Omega(H)_n$ is the n th harmonic of $\Omega(H)$. It should be recalled that the above expression is only valid for $\alpha(H) < 0$. When we are deep enough into the superconducting state so that we are away from the reentrance region we have $a_1(H_{c2}/H - 1) > a_2$. This means $3a_2^2g_2/4g_1^2 \ll a_2^2/g_1 < (a_1a_2/g_1)(H_{c2}/H - 1)$ and we can neglect the small constant term $3a_2^2g_2/g_1^2$. We thus get the following form for the first harmonic of the grand potential:

$$\Omega_{S1} = \Omega_{N1} + (\Omega_S - \Omega_N)_1, \quad (29)$$

where³⁰

$$\Omega_{N1} = -\frac{eL_xL_yH}{2\pi\hbar c} \frac{\hbar\omega_c}{\pi^2} \left[4\pi^2 \frac{k_B T}{\hbar\omega_c} e^{-2\pi^2(k_B T/\hbar\omega_c)} \right] \times \cos(2\pi\mu/\hbar\omega_c). \quad (30)$$

We have written the reduction due to finite temperature in square brackets.

$$\hbar\omega_c \sum_{n_1, n_2} B_0^{n_1, n_2} \frac{\tanh(\beta\xi_{n_1}/2) + \tanh(\beta\xi_{n_2}/2)}{\xi_{n_1} + \xi_{n_2}} w^2(n_1)w^2(n_2) = \sum_{l, m} e^{2\pi i n_f(m-l)} \int dx \int dy e^{2\pi i(mx - ly)} \frac{e^{-(x-y)^2/4n_f} \tanh(\beta\xi_x/2) + \tanh(\beta\xi_y/2)}{\sqrt{\pi n_f} (x+y)} w^2(x)w^2(y) = \sum_{l, m} I_{l, m} e^{2\pi i n_f(m-l)}, \quad (32)$$

where $\xi_x = \hbar\omega_c x$ and $w(x) = e^{-(\xi_x/0.5\hbar\omega_D)^2} = e^{-x^2/\sigma^2}$. To estimate $I_{l, m}$ where $(l, m) \neq (0, 0)$ we write the integral in the form

$$I_{l, m} = \frac{2k_B T}{\hbar\omega_c} \sum_{\nu} \int dx \int dy \frac{e^{-(x-y)^2/4n_f} e^{-2(x^2+y^2)/\sigma^2 + 2\pi i(mx - ly)}}{\sqrt{\pi n_f} (x - i\omega'_{\nu})(y + i\omega'_{\nu})}, \quad (33)$$

where $\omega'_{\nu} = \omega_{\nu}/\omega_c$. The first harmonic of $\alpha(H)$ comes from the terms with $|l - m| = 1$. Taking $m = 1$ and $l = 0$ yields the integral

$$\int dx \frac{e^{2\pi i x - 2x^2/\sigma^2}}{x - i\omega'_{\nu}} \int dy \frac{e^{-2y^2/\sigma^2 - (x-y)^2/4n_f}}{y + i\omega'_{\nu}}. \quad (34)$$

We approximate this integral by

$$\int dx \frac{e^{2\pi i x}}{x - i\omega'_{\nu}} \int dy \frac{e^{-(y-x)^2/4n_f}}{y + i\omega'_{\nu}}, \quad (35)$$

since we have assumed $8n_f \ll \sigma^2$. The integral can be solved exactly and we get

B. Calculation of the oscillatory terms

In this section we will derive some approximate expressions for the coefficients a_2 and g_2 . We are interested in how a_2 and g_2 depend on the parameters n_f , ω_D , and T . It turns out that it is fairly straightforward to extract this dependence for the oscillatory terms. First we note the following approximate identity coming from the law of large numbers:

$$B_0^{n_1, n_2} \simeq \frac{1}{\sqrt{4\pi n_1}} e^{-(n_1 - n_2)^2/8n_1} \simeq \frac{1}{\sqrt{4\pi n_f}} e^{-(n_1 - n_2)^2/8n_f}, \quad (31)$$

where we have assumed that $|n_1 - n_2|/n_1 \ll 1$ and $n_1 \simeq n_f$ (i.e., $\omega_D/\omega_c \equiv 2\sigma \ll n_f$). Using this formula, Eq. (11), and the Poisson identity we get the following integrals for $\alpha(H)$:

$$I_{0,1} = \frac{4k_B T \pi^2}{\hbar\omega_c \sqrt{\pi n_f}} \sum_{\nu \geq 0} e^{-2\pi\omega'_{\nu}} [1 - \Phi(\omega'_{\nu}/\sqrt{n_f})] e^{\omega'_{\nu} 2/n_f} + e^{t^2} [1 - \Phi(t)] e^{-4\pi^2 n_f} \simeq \frac{4k_B T}{\hbar\omega_c \sqrt{\pi n_f}} \pi^2 e^{-2\pi^2 k_B T/\hbar\omega_c} \simeq \frac{4k_B T}{\hbar\omega_c \sqrt{\pi n_f}} \pi^2 e^{-2\pi^2 k_B T/\hbar\omega_c}, \quad (36)$$

where $\Phi(x) \equiv 2\pi^{-1/2} \int_0^x e^{-s^2} ds$ is the error function and $t = (\omega' + 2\pi n_f)/\sqrt{n_f}$. Here we have used that $\exp(-2\pi\omega'_{\nu \neq 0}) \ll \exp(-2\pi\omega'_{\nu=0})$ for $2\pi^2 k_B T/\hbar\omega_c \geq 1$, $\exp(-4\pi^2 n_f) \ll 1$, and $n_f^{-1/2} \omega_{\nu=0} \ll 1$. So in this temperature range the dominant contribution to the first harmonic comes from the lowest Matsubara frequency, which makes our approximation above self-consistent. The contribution to the first harmonic from the $|l - m| = 1$ term given $l, m \neq 0$ can be calculated in the same way; it is proportional to $\exp(-2\pi^2 k_B T/\hbar\omega_c)$ and therefore negligible for $2\pi^2 k_B T/\hbar\omega_c \geq 1$, in agreement with the results obtained by Gruenberg and Gunther.⁹ After some algebra, the calculations outlined above combined with Eq. (11) lead to the following approximate result:

$$a_2 \simeq \frac{V^2(a_x/l) 2\pi}{L_x L_y l^2 \sqrt{\pi n_f}} \frac{k_B T}{(\hbar\omega_c)^2} e^{-2\pi^2 k_B T/\hbar\omega_c}. \quad (37)$$

The above result that a_2 is proportional to $1/\sqrt{n_f}$ and $k_B T e^{-2\pi^2 k_B T/\hbar\omega_c}$ and independent of ω_D is still correct even

when $\sigma^2 \ll 8n_f$, as long as $\min(\sigma, \sqrt{n_f}) \gg 1$ and $2\pi^2 k_B T / \hbar \omega_c \geq 1$. Inclusion of spin is equivalent to making the substitution $x \rightarrow x + gm^*/4m_0$ and $y \rightarrow y - gm^*/4m_0$ in the integrals $I_{l,m}$. This results in a reduction factor $\cos(\pi gm^*/2m_0)$ in Eq. (37) if $\min(\sqrt{n_f}, \sigma) \gg g$.

The calculations for g_2 are very similar to the ones above. Using Eq. (12) and the Poisson formula we end up with the following integrals determining the dependence of γ on n_f , T , and ω_D :

$$\sum_{l_1, l_2, l_3, l_4} \frac{k_B T}{n_f} e^{2\pi i n_f (l_1 + l_3 - l_2 - l_4)} dx_1 \cdots dx_4 \frac{e^{[(x_1 - x_4)^2 + (x_3 - x_2)^2 + (x_1 - x_2)^2 + (x_3 - x_4)^2]/8n_f}}{(i\omega'_v - x_1)(i\omega'_v + x_2)(i\omega'_v - x_3)(i\omega'_v + x_4)} \times e^{-2(x_1^2 + x_2^2 + x_3^2 + x_4^2)/\sigma^2} e^{2\pi i (l_1 x_1 + l_3 x_3 - l_2 x_2 - l_4 x_4)} \Xi_{x_1 + x_2, x_3 + x_4}^{x_1 + x_4, x_2 + x_3} \quad (38)$$

where $\Xi_{j_3, j_4}^{j_1, j_2}$ is given in Eq. (14). Contributions to the first harmonic g_2 come from the terms with $|l_1 + l_3 - l_2 - l_4| = 1$. As in the case for a_2 we can neglect the terms with more than one l_i different from zero when $2\pi^2 k_B T / \hbar \omega_c \geq 1$. Although we do not have any simple expression for $\Xi_{x_1 + x_2, x_3 + x_4}^{x_1 + x_4, x_2 + x_3}$, we can still extract the dependence on T , ω_D , and n_f . This is because the integral over $x_2 \cdots x_4$ does not vary appreciably with x_1 on a scale $\approx \omega'_v = 0$. Using the result $\int dx [\exp(2\pi i x_1) / (i\omega' - x_1)] f(x_1) \propto f(0) e^{-2\pi\omega'}$ ($\omega' > 0$) for any well-behaved function $f(x)$ which varies slowly for $x \leq \omega'$ and taking $l_1 = 1$, $l_2 = l_3 = l_4 = 0$ we get the integral

$$\frac{k_B T}{n_f} dx_1 \frac{e^{2\pi i x_1}}{i\omega'_v - x_1} dx_2 \cdots dx_4 \frac{e^{[x_4^2 + (x_3 - x_2)^2 + x_2^2 + (x_3 - x_4)^2]/8n_f}}{(i\omega'_v + x_2)(i\omega'_v - x_3)(i\omega'_v + x_4)} e^{2(x_2^2 + x_3^2 + x_4^2)/\sigma^2} \Xi_{x_2, x_3 + x_4}^{x_4, x_2 + x_3} \quad (39)$$

The factors $1/(i\omega' \pm x_j)$ in the integrand make the integral largely independent of any long-range behavior determined by σ and n_f as long as $|\omega'| \ll \min(\sigma, \sqrt{n_f})$. We therefore conclude that g_2 is independent of ω_D and that it only depends on n_f through the n_f^{-1} -factor coming from the four $B_0^{N,M}$ coefficients. We also obtain that g_2 is proportional to $k_B T \exp(-2\pi^2 k_B T / \hbar \omega_c)$. The proportionality constant is found through an exact evaluation of γ given in Eq. (12). We obtain

$$g_2 \approx \frac{(V/\hbar \omega_c)^{4/27}}{n_f (L_x L_y)^3 l^2} k_B T e^{-2\pi^2 k_B T / \hbar \omega_c} \quad (40)$$

Again the effect of spin (i.e., nonzero g factor) provide an additional $\cos(\pi gm^*/2m_0)$ in Eq. (40). It is not surprising that the oscillatory terms a_2 and g_2 are independent of the pairing width ω_D since the oscillations are a consequence of the individual Landau levels going through the chemical potential. Likewise the $1/\sqrt{n_f}$ and $1/n_f$ dependence reflects the fact that the probability for two electrons, each with energy $(n + 1/2)\hbar \omega_c$, to form a pair with minimum center-of-mass energy is proportional to $1/\sqrt{n}$ for high quantum numbers, as can be seen from Eq. (31). This proportionality can be explained via simple phase-space considerations. We have tested the dependence of a_2 and g_2 on the different parameters n_f , ω_D , and T and we find excellent agreement with our approximate forms.

To facilitate comparison with earlier papers we will now formally treat the order parameter $\Delta(\mathbf{r})$ as a free parameter and assume that the oscillatory behavior of Eq. (18) only comes from the harmonics of the expansion coefficients α , γ , etc. This is of course incorrect since the self-consistent order parameter itself is an oscillatory function of

the field, making the results where the corrections to the harmonics of the dHvA oscillations due to superconductivity are expressed as a power series in Δ (Refs. 11, 12 and 31) of limited validity. However, to compare with the earlier predictions we ignore for the moment the oscillations in Δ_0 and treat it formally as a free parameter [i.e., $(\Omega_S - \Omega_N)_1 = a_2 \Delta_0^2 - g_2 \Delta_0^4 + \cdots$]. Here we focus on the Δ^4 term since there are discrepancies between the predictions of different authors for this term. Since

$$\Delta^2 \equiv (L_x L_y)^{-1} \int d\mathbf{r} |\Delta(\mathbf{r})|^2 = \frac{V^2 a_x}{\sqrt{2} L_x^2 L_y^2 l} \Delta_0^2, \quad (41)$$

we obtain using Eqs. (40) and (30) the formal result for the fourth-order term:

$$(\Omega_S - \Omega_N)_1 |_{\Delta^4 \text{ term}} = -g_2 \Delta_0^4 \approx \Omega_{N1} \frac{10}{n_f} \left(\frac{\Delta}{\hbar \omega_c} \right)^4. \quad (42)$$

Stephen¹² obtained $\sim 16 \Omega_{N1} / n_f (\Delta / \hbar \omega_c)^4$ for the same quantity using a different semiclassical approach. The n_f dependences of the two result agree but the numerical prefactors are somewhat different. The above arguments for the n_f dependence of g_2 can easily be generalized yielding that the n_f dependence of the first harmonic of the Δ^{2n} term is $n_f^{-n/2}$. This n_f dependence agrees with the result obtained by Stephen whereas it disagrees with the $n_f^{-3/2}$ dependence for the Δ^4 term obtained by Maniv *et al.*³¹ We cannot over-emphasize the fact that the above scheme to calculate the damping of the oscillations due to superconductivity is incorrect, since it ignores the oscillations in Δ as a function of the

field. To include those we have to use a self-consistent order parameter and hence Eq. (28).

One debated issue is the possibility of reentrance for type-II superconductors.¹⁰ The oscillatory behavior of α due to the Landau level structure gives rise to the possibility of several solutions to $\alpha(H)=0$ for a given temperature. This should be reflected in a highly oscillatory behavior of the transition line $H_{c2}(T,H)$. Such an oscillatory behavior has never been observed experimentally. Using the approximate expressions for a_1 and a_2 we can estimate the temperature below which there is reentrance and such oscillations in H_{c2} should occur in a two-dimensional metal. We obtain that when there is no impurity scattering, no Zeeman splitting, and $n_f \sim O(10^2)$ one should observe these oscillatory effects in H_{c2} in a 2D metal for temperatures lower than $k_B T / \hbar \omega_c \approx 0.3$. However, inclusion of spin reduces the amplitude of the oscillations of α by a factor $\cos(\pi g m^*/2m_0)$ close to the transition line. Assuming that impurities reduces the oscillations by a factor $\exp(-2\pi^2 k_B T_D / \hbar \omega_c)$ where T_D is the Dingle temperature we obtain that there will not be any reentrance if $k_B T_D / \hbar \omega_c \approx 0.2$ no matter how low the temperature is. In the case of the experiments being done on κ -(ET)₂Cu(NCS)₂ (Ref. 2) the experimental parameters are such that $k_B T_D / \hbar \omega_c \approx 0.27$ and $|\cos(\pi g m^*/2m_0)| \approx 0.3$. They will therefore never observe these reentrance effects. The magnetic oscillations in the thermodynamic quantities will of course still be there since α and γ are still oscillatory.

C. Approximate results for damping

In this section we will draw some conclusions from the general form of the damping of the dHvA oscillations due to the growth of the superconducting order described by Eq. (28). The first thing we notice is that in this approximation the superconducting damping has a simple polynomial form in $(H_{c2}/H-1)$. The damping is maximum for $(H_{c2}/H-1) = a_2 g_1 / a_1 g_2$. For $(H_{c2}/H-1) > a_2 g_1 / a_1 g_2$ the damping decreases when we go deeper into the superconducting state and for $(H_{c2}/H-1) > 2a_2 g_1 / a_1 g_2$ the magnetic oscillations are enhanced by the superconducting order. This explains the observations made in Sec. III. The in-phase oscillations between the fourth-order $\Omega_S - \Omega_N$ and Ω_N are due to the oscillatory behavior of $\gamma(H)$. Since $\gamma(H)$ oscillates in phase with Ω_N , we will get the enhancement of the oscillations of Ω_S compared to Ω_N when the smooth part of $\alpha(H)$ is sufficiently large. Again we must emphasize that this is obviously a sign that our perturbative scheme has broken down and does not reflect any physical effect.

To make any quantitative predictions we need to use our approximate expressions for a_i and g_i . Since we only have very good approximations for a_2 and g_2 and for the temperature and spin dependence of a_1 and g_1 , we will concentrate on properties that can be derived from these results. From Eq. (28) and the temperature dependence of a_i and g_i we conclude that the first harmonic of the condensation energy $(\Omega_S - \Omega_N)_1$ is proportional to $k_B T \exp(-2\pi^2 k_B T / \hbar \omega_c)$. Since we also have $\Omega_N \propto k_B T \exp(-2\pi^2 k_B T / \hbar \omega_c)$, this means that the magnetic oscillations have the same temperature dependence in the mixed state as in the normal state. This result agrees with the general theory (see Schoenberg,³⁰ Sec. 2.5 and Sec. 2.3) valid for any part of the grand potential which

is proportional to $\cos(\mu/\hbar\omega_c)$. It is also confirmed by experimental observations.³² Likewise the effect of spin on $(\Omega_S - \Omega_N)_1$ is a reduction in the amplitude by a factor $\cos(\pi g m^*/2m_0)$. This is the same reduction factor as for the oscillations in the normal state.³⁰ We thus have no extra damping effects due to spin close to the transition line where the perturbation theory is valid.

We can now examine whether the arguments based on the Gor'kov expansion leading to a sign change of the first harmonic are valid. Naively one would expect a sign change since the contribution from the condensation energy to the magnetic oscillations is in antiphase with the normal-state oscillations. When the system is deep enough into the mixed state the superconducting oscillations would dominate leading to a sign change of the magnetic oscillations. Extrapolating the rate of the damping close to H_{c2} obtained from the Gor'kov expansion Maniv and Rom¹⁸ have estimated the magnetic field $H_{inv} < H_{c2}$ at which this sign change should occur. We are now able to show that this argument based on the perturbative expansion of the grand potential is incorrect. From Eq. (28) we obtain that the maximum amplitude of the antiphase oscillations of $\Omega_S - \Omega_N$ is given by $a_2^2/4g_2$. Using our approximate expressions for a_2 and g_2 we get

$$\frac{a_2^2}{4g_2} \approx \frac{L_x L_y a_x^2 \pi}{l^4 27} k_B T e^{-2\pi^2 k_B T / \hbar \omega_c}. \quad (43)$$

Comparing this amplitude with the contribution from the normal-state oscillations given in Eq. (30) we see that our perturbation scheme roughly predicts a maximum damping of 50%. It must be emphasized that this does not mean that the damping of the model described by the Hamiltonian in Eq. (3) has a maximum of 50%. However, using the result above combined with the results in Sec. III, we can conclude that neither the argument based on the Gor'kov expansion nor the arguments based on a simplified form for the quasi-particle spectrum leading to an inversion of the first harmonic of the dHvA signal are valid.

VI. COMPARISON WITH EXPERIMENT

In this section we present a typical result for the damping of the magnetic oscillations obtained from our theory when many Landau levels participate in the pairing. We have chosen parameters such that we can compare our result with the experimental observations made by van der Wel *et al.*² First we compare our approximate expressions for the damping from Eq. (28) with the result based on the exact evaluation of α and γ from Eq. (11) and Eq. (12). We used the set of parameters such that $k_B T / \hbar \omega_c = 0.25$, $V / \hbar \omega_c = 2.315$, and $\omega_D / \omega_c = 75$ when $n_f = 175$. There is no Zeeman effect and the chemical potential is conserved. In Fig. 6 we have plotted the magnetization for both the normal state and the mixed state calculated from the perturbative expansion to fourth order as a function of n_f . The perturbation theory predicts a substantial damping of the oscillations over many periods, reaching a maximum for $n_f \approx 170$. At the maximum the first harmonic is damped approximately 50% in agreement with the result in the previous section. As we go deeper into the mixed state, the damping decreases according to the perturbative scheme. Based on the results in Sec. III, we expect the

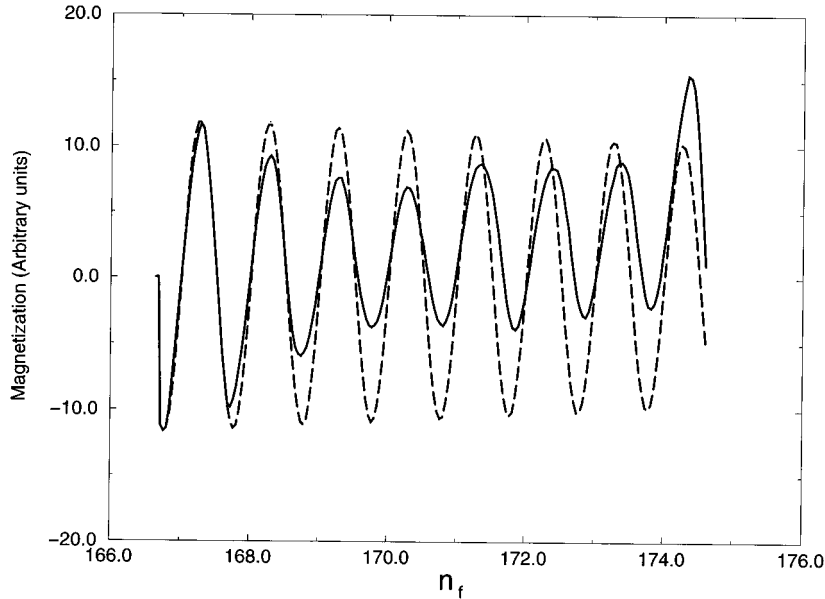


FIG. 6. The magnetization vs n_f in the mixed state (solid line) and in the underlying normal state (dashed line).

perturbation theory to describe the damping well for $n_f \lesssim 170$. Due to the large number of Landau levels involved in pairing, we have not undertaken the exact numerical calculation for this set of parameters. In Fig. 7 we have plotted M_s calculated from the exact evaluation of $\alpha(H)$ and $\gamma(H)$ and calculated from Eq. (28). We see that the simplified expression reproduces the perturbative predictions well.

The above parameters approximate the experiment performed by van der Wel *et al.*² on the essentially 2D organic superconductor κ -(ET)₂Cu(NCS)₂. To compare with the experimental data we will formulate our results in terms of a field-dependent quasiparticle scattering rate τ defined such that $e^{-\pi/\omega_c\tau}$ gives the damping of the first harmonic of the dHvA oscillations due to superconductivity. From Eq. (29) we get

$$\tau^{-1} = -\frac{\omega_c}{\pi} \ln[1 + (\Omega_S - \Omega_N)_1 / \Omega_{N1}]$$

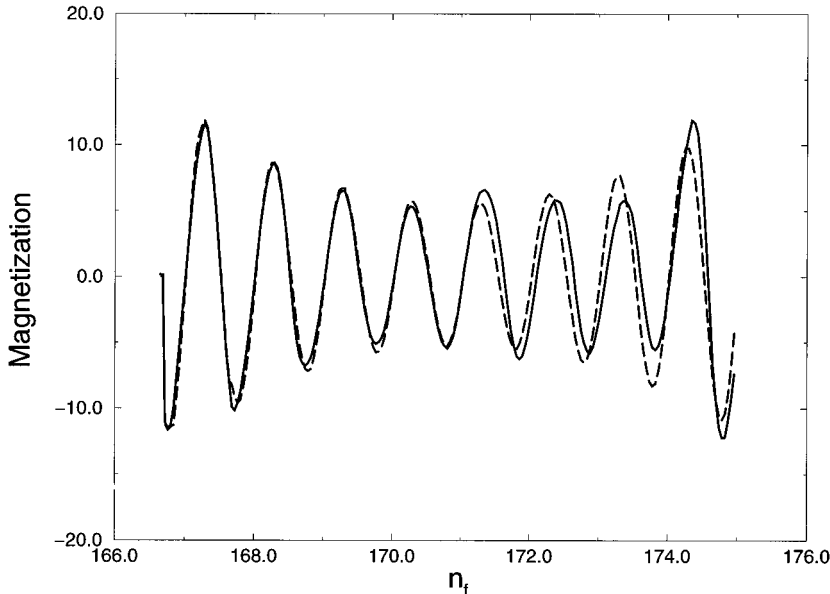


FIG. 7. The magnetization vs n_f in the mixed state. The solid line is the first harmonic of the perturbative calculation and the dashed line is obtained from Eq. (28).

$$\approx -\frac{\omega_c a_1 a_2}{2\pi g_1 \Omega_{N1}} (H_{c2}/H - 1), \quad (44)$$

where we have used Eq. (28). The approximate equality is only valid for $a_2 g_1 / a_1 g_2 \ll H_{c2}/H - 1$. Using the expressions for a_i , g_i , and Ω_{N1} we can now compare this expression with the experimental observations. Unfortunately the experimental value of H_{c2} is uncertain. The transition from the normal state to the superconducting state occurs over a field range of approximately $2T$.³³ This gives a “smooth” variation of the τ^{-1} on entering the mixed state which our theory cannot account for. To model this transition region we use the method introduced in Ref. 2 by including a Gaussian spread in H_{c2} . In Fig. 8 we have plotted the experimental data for τ^{-1} (bars) measured in (THz) as a function of $1/B$ measured in T^{-1} . The solid line is our theoretical prediction based on Eq. (44) including a Gaussian spread in H_{c2} . The agreement between theory and experiment is good. It should

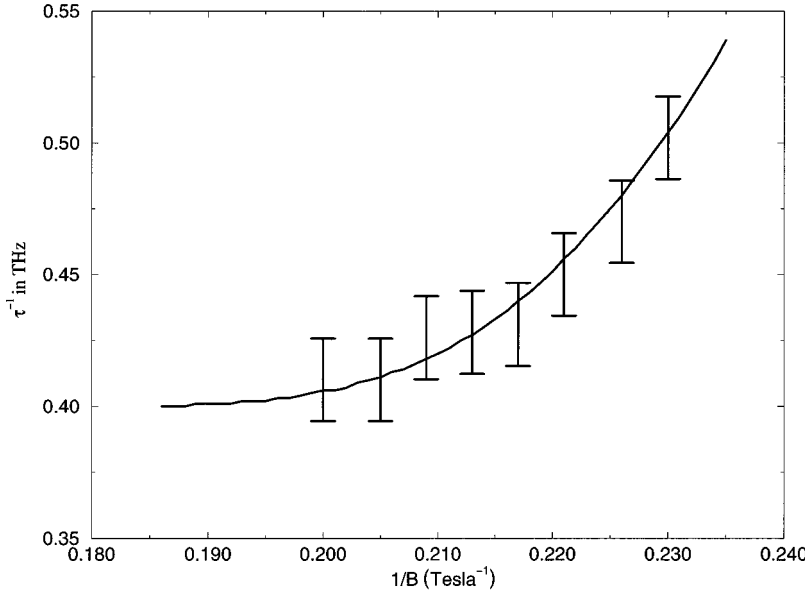


FIG. 8. τ^{-1} as a function of $1/B$. The solid line is the theoretical prediction and the bars are the experimental data (Ref. 2).

be noted that we have no fitting parameters apart from H_{c2} . However, without a more reliable measurement of H_{c2} a precise comparison between our theory and the experimental observations cannot be made.

VII. CONCLUSION

In this paper we have examined the dHvA oscillations in the mixed state of a type-II superconductor in the 2D limit using both a numerical solution of the BdG equations and an analytical theory based on a self-consistent Gor'kov expansion. The use of translational and rotational symmetry has simplified the analysis such that we have been able to calculate the expansion coefficients exactly to any order without using semiclassical or other approximations. Comparison with the exact numerical solution has showed that perturbation theory works well close to H_{c2} , thereby disproving recent claims of nonperturbative effects. We have found that the condensation energy oscillates in antiphase with the normal grand potential, thus producing damping of the dHvA oscillations in agreement with numerical and experimental results. The damping is directly connected with the enhancement of superconductivity when we have a Landau level at the chemical potential. We have excluded the possibility of a sign change of the first harmonic of the dHvA oscillations in the mixed state. The effect of spin and a conserved number of particles as opposed to a conserved chemical potential was examined. Using a simple approximate form of our analytical theory valid when many Landau levels participate in pairing we have compared our theory with an experiment on the quasi-2D organic superconductor κ -(ET)₂Cu(NCS)₂. We have found good agreement. However, due to experimental uncertainty about H_{c2} any quantitative comparison is impossible.

ACKNOWLEDGMENTS

We would like thank J. Singleton and S. Hayden for many helpful discussions. This work has been supported in part by EPSRC Grant No. GR/K 15619 (V.N.N. and N.F.J.) and by The Danish Research Academy (G.M.B.).

APPENDIX A

Using the symmetry of the vortex lattice and making the restriction $\Delta_{j \neq 0} = 0$ we obtain

$$\begin{aligned} \Omega_6 = & -\frac{V^6 a_x^6}{24(L_x L_y)^6} \Delta_0^6 \sum_{n_1 \dots n_6} f(n_1, \dots, n_6) \\ & \times B_0^{n_1 n_2} B_0^{n_3 n_4} B_0^{n_5 n_6} B_0^{n_5 n_4} B_0^{n_3 n_2} \\ & \times B_0^{n_1 n_6} \Xi_{n_5+n_4, n_3+n_2, n_1+n_6}^{n_1+n_2, n_3+n_4, n_5+n_6} \end{aligned} \quad (\text{A1})$$

where

$$\begin{aligned} f(n_1, n_2, \dots, n_{2l}) = & \frac{1}{\beta} \sum_{\nu} [(-i\hbar\omega_{\nu} - \xi_{n_1\downarrow}) \\ & \times (i\hbar\omega_{\nu} - \xi_{n_2\uparrow}) \dots (i\hbar\omega_{\nu} - \xi_{n_{2l}\uparrow})]^{-1} \end{aligned} \quad (\text{A2})$$

and

$$\Xi_{j_1, \dots, j_{2l}}^{j_1, \dots, j_l} = \sum_{\mathbf{k} \in MBZ} \chi_{j_1}(\mathbf{k}) \dots \chi_{j_l}(\mathbf{k}) \chi_{j_{l+1}}^*(\mathbf{k}) \dots \chi_{j_{2l}}^*(\mathbf{k}), \quad (\text{A3})$$

$$\chi_j(\mathbf{k}) = \sqrt{l} \sum_b e^{2ik_x a_x b} e^{-i\pi b^2/2} \phi_j[\sqrt{2}(k_y l + b a_x/l)]. \quad (\text{A4})$$

Likewise the eighth-order term gives for $\Delta_{j \neq 0} = 0$

$$\begin{aligned} \Omega_8 = & \frac{V^8 a_x^8}{64(L_x L_y)^8} \Delta_0^8 \sum_{n_1 \dots n_8} f(n_1, \dots, n_8) \\ & \times B_0^{n_1 n_2} B_0^{n_3 n_4} B_0^{n_5 n_6} B_0^{n_7 n_8} B_0^{n_7 n_6} B_0^{n_5 n_4} B_0^{n_3 n_2} \\ & \times B_0^{n_1 n_8} \Xi_{n_7+n_6, n_5+n_4, n_3+n_2, n_1+n_8}^{n_1+n_2, n_3+n_4, n_5+n_6, n_7+n_8}. \end{aligned} \quad (\text{A5})$$

The Matsubara sums and the \mathbf{k} sums can be calculated as in the fourth-order case.

APPENDIX B

In this appendix we will extract the dependence of a_1 and g_1 on n_f , T , σ , and spin. This is considerably harder than for a_2 and g_2 because we do not have any oscillatory factor in the integrals that would make the long-range behavior of the remaining integrand insignificant. It turns out that it is still fairly straightforward to derive the temperature and spin dependence of a_1 and g_1 , whereas we have to make some rather drastic approximations to obtain the dependence on n_f and σ for g_1 .

The smooth part (zero harmonic) of $\alpha(H)$ comes from the terms $I_{l,l}$ in Eq. (32). We first look at the term $l=m=0$. Making the variable substitution $v=(x+y)/\sigma\sqrt{2}$, $u=(x-y)/\sigma\sqrt{2}$ we get the following integral:

$$I_{0,0} = \frac{\sigma}{\sqrt{2\pi n_f}} \int du \int dv e^{-(\sigma^2/2n_f+2)u^2} \{ \tanh[K\sigma(v+u)] + \tanh[K\sigma(v-u)] \} \frac{e^{-2v^2}}{v}, \quad (\text{B1})$$

where $K = \beta\hbar\omega_c/2\sqrt{2} \gg 1$ determines the temperature dependence of the integral. Since K is only important around the region $v \approx 0$ which does not contribute significantly to the integral, we conclude that $I_{0,0}$ is independent of the temperature to a very good approximation. Since similar calculations to the ones in Sec. V B show that for $2\pi^2 k_B T / \hbar\omega_c \geq 1$ we can neglect the contribution to the zero harmonic from the $I_{l,l}$ terms where $l \neq 0$, we conclude that a_1 for is independent of the temperature for temperatures that are not too low. We

have checked this independence against the exact result given in Eq. (11) and found very good agreement. To obtain the dependence on n_f and σ we make the simplification

$$\tanh[K\sigma(v+u)] + \tanh[K\sigma(v-u)] v^{-1} \approx \begin{cases} 0 & \text{if } |v| < |u|, \\ \frac{2}{|v|} & \text{if } |v| > |u|, \end{cases} \quad (\text{B2})$$

which is a very good approximation since $K \gg 1$. It is exact for $T=0$. The integral can be solved and we obtain

$$I_{0,0} \approx \frac{4}{\sqrt{1+n_f/\sigma^2}} \ln \left(\sqrt{\frac{\sigma^2}{4n_f} + 1} + \sqrt{\frac{\sigma^2}{4n_f} + 2} \right) \approx 2 \ln \left(\frac{\sigma^2}{n_f} \right), \quad (\text{B3})$$

where we have assumed $\sigma^2 \gg 4n_f$. This yields the result

$$a_1 \approx \frac{V^2(a_x/l)}{4\pi L_x L_y l^2 \hbar \omega_c}. \quad (\text{B4})$$

The expression for a_1 is independent of any spin effects for $\min(\sqrt{n_f}, \sigma) \gg g$. We have again checked the independence of a_1 on n_f , σ , and spin against the exact result and we find very good agreement.

The dependence of g_1 on n_f , σ , and T is determined by the integrals in Eq. (38) for which $l_1 - l_2 + l_3 - l_4 = 0$. Again it turns out that for $2\pi^2 k_B T / \hbar\omega_c \geq 1$ we can neglect the contribution to g_1 from the terms with $l_1 - l_2 + l_3 - l_4 = 0$ and $\max(|l_1|, |l_2|, |l_3|, |l_4|) > 0$. Using Eq. (16) we can rewrite the integral with $l_1 = l_2 = l_3 = l_4 = 0$ as

$$\int dx_1 \cdots dx_4 \frac{\hbar\omega_c}{2} \left[\frac{1}{x_3 - x_1} \left(\frac{\tanh(Kx_1/2)}{(x_1+x_2)(x_1+x_4)} - \frac{\tanh(Kx_3/2)}{(x_3+x_2)(x_3+x_4)} \right) + \frac{1}{x_4 - x_2} \left(\frac{\tanh(Kx_2/2)}{(x_1+x_2)(x_2+x_3)} - \frac{\tanh(Kx_4/2)}{(x_4+x_1)(x_4+x_3)} \right) \right] e^{[(x_1-x_4)^2 + (x_3-x_2)^2 + (x_1-x_2)^2 + (x_3-x_4)^2] / 8n_f} e^{-2(x_1^2+x_2^2+x_3^2+x_4^2)/\sigma^2} \Xi_{x_1+x_2, x_3+x_4}^{x_1+x_4, x_2+x_3} \quad (\text{B5})$$

where $K = \hbar\omega_c/k_B T$ determines the temperature dependence. Again for $\min(\sqrt{n_f}, \sigma) \gg g$, g_1 will be independent of spin effects. As in the case of a_1 , it is fairly straightforward to see that since $1/K \ll \min(\sqrt{n_f}, \sigma)$, the integral and therefore g_1 are independent of the temperature to a very good approximation. We have checked this independence against the exact result given in Eq. (12) and find very good agreement.

To make any progress in determining the dependence of g_1 on σ and n_f we need some simple expression for $\Xi_{n_1+n_2, n_3+n_4}^{n_1+n_4, n_2+n_3}$. As a rough approximation we make the simplification to

$$\Xi_{n_1+n_2, n_3+n_4}^{n_1+n_4, n_2+n_3} \sim (\delta_{n_1, n_3} + \delta_{n_2, n_4}) \frac{L_x L_y}{4\pi a_x^2}. \quad (\text{B6})$$

This is based on the fact that $\chi_{j_1}(\mathbf{k}) \chi_{j_2}^*(\mathbf{k})$ in general is a complex number for $j_1 \neq j_2$. When the \mathbf{k} sum is performed

the phase factor will change ‘‘randomly’’ and make the sum approximately zero. Physically it corresponds to ignoring cases where electrons in four different Landau levels interact. Using this simplification, Eq. (31), and the Poisson formula we get from Eq. (12) the following integral determining the dependence of g_1 on n_f and σ :

$$\sum_{\omega'} \frac{k_B T}{n_f} \int dx dx_2 dx_4 e^{-[(x-x_2)^2 + (x-x_4)^2] / 4n_f} \times \frac{e^{-2(x^2+x_2^2+x_4^2)/\sigma^2}}{(i\omega' - x)^2 (i\omega' + x_2) (i\omega' + x_4)} e^{-2(2x^2+x_2^2+x_4^2)/\sigma^2} = \sum_{\omega'} I_{\omega'}, \quad (\text{B7})$$

where $\omega' = \omega_v / \omega_c$. We have again assumed $2\pi^2 k_B T / \hbar\omega_c \geq 1$. Assume now that $8n_f \ll \sigma^2$. We approximate the integrals by

$$I_{\omega'} \approx \frac{k_B T}{n_f} \int dx \frac{e^{-x^2/2n_f}}{(i\omega' - x)^2} \int dx_2 \frac{e^{-x_2^2/4n_f}}{i\omega' + x_2} \int dx_4 \frac{e^{-x_4^2/4n_f}}{i\omega' + x_4}. \quad (\text{B8})$$

We will now show that in this approximation the sum of the integrals is largely independent of n_f and therefore $g_1 \propto 1/n_f$. The integral can be solved and we get

$$I_{\omega'} = \frac{k_B T}{n_f^{3/2}} \left\{ -\frac{\pi |\omega'|}{\sqrt{n_f}} e^{\omega'^2/2n_f} \left[1 - \Phi \left(\frac{|\omega'|}{\sqrt{2n_f}} \right) \right] + \sqrt{2\pi} \right\} \pi^2 \times \left[1 - \Phi \left(\frac{|\omega'|}{2\sqrt{n_f}} \right) \right]^2 e^{\omega'^2/2n_f}, \quad (\text{B9})$$

where we again have $\Phi(x) \equiv (2/\sqrt{\pi}) \int_0^x dt e^{-t^2}$. Equation (B7) can then be written on the form

$$\frac{\hbar \omega_c}{2\pi n_f} \Delta x \sum_{x_n} \left\{ -\pi x_n e^{x_n^2/2} \left[1 - \Phi \left(\frac{x_n}{\sqrt{2}} \right) \right] + \sqrt{2\pi} \right\} \pi^2 \times \left[1 - \Phi \left(\frac{x_n}{2} \right) \right]^2 e^{x_n^2/2}, \quad (\text{B10})$$

where $x_n = \Omega_N / \omega_c \sqrt{n_f}$ and $\Delta x = 2\pi k_B T / \hbar \omega_c \sqrt{n_f}$. Since $\Delta x \ll 1$, we can approximate this sum by an integral and we therefore conclude that g_1 is independent of the temperature in agreement with the result above. Furthermore, we obtain $g_1 \propto 1/n_f$ for n_f large and g_1 independent of σ . When $\sigma^2 \gg 8n_f$ does not hold the calculation is the same as above. We just have to substitute $1/4n_f$ with $1/4n_f + 2/\sigma^2$ in the integrals. The $1/n_f$ dependence coming from the $B_0^{j_1 j_2}$ factors in Eq. (12) is unaltered and we still get that $g_1 \propto 1/n_f$ for $\min(\sqrt{n_f}, \sigma)$ large and that g_1 is independent of σ and the temperature. By calibrating g_1 through an exact evaluation based on Eq. (12), we obtain

$$g_1 \approx \frac{V^4}{(L_x L_y)^3 l^2 (\hbar \omega_c)^3 5.4 n_f}, \quad (\text{B11})$$

where g_1 is defined in Sec. V A. It should be noted that the dependence of g_1 on n_f and σ in the above expression is only approximate and rests on the various simplifications made. We have tested the above expression against the exact result and we find that the dependence on n_f and σ fits to an accuracy of 20%.

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