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LETTER TO THE EDITOR

A unified mean field approach to the dHvA effect in the vortex state near the upper critical field

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Abstract. The effect of nonmagnetic impurity scattering on the additional damping of de Haas–van Alphen (dHvA) oscillations in the mixed state of type II superconductors near the upper critical field is studied within mean field theory in the relaxation time approximation. Our calculations show that this effect becomes important only for small thermal smearing of the single particle distribution function and small disorder broadening of the Landau levels. The relationships between the different mechanisms of broadening are discussed.

The theory of the magnetic quantum oscillations observed experimentally in the mixed state of several type II superconductors (SC) has been recently reviewed [1]. The variety of microscopic models for the description of the experimental data in the close vicinity of the upper critical field, H_{c2} , reflects a lack of a unified approach which could establish relationships between the proposed models and could determine the different ranges of their validity.

Specific conditions characterize all models. The Maki–Stephen (MS) [2] semi-classical model, which was also derived by Wasserman and Springford using an alternative approach [3], not only neglects the coherence of the quasi-particle scattering by the vortex lattice [4], but also does not take into account properly the Landau level (LL) broadening effect due to impurity scattering and the smearing of the quasi-particle distribution function due to thermal excitations. In the semi-classical approach, developed in [4] and [5] on the basis of perturbation expansion in the order parameter for a pure two-dimensional (2D) SC, the thermal excitations were taken into account exactly. However, it was shown by these studies that the Gorkov expansion fails to describe the low temperature limit because of the infinite degeneracy of the Landau levels (LL).

Numerical simulations [6, 7] of the corresponding Bogoliubov–de Gennes equations in this limit led to a linear dependence of the damping rate on the order parameter Δ_0 , which cross-overs to MS-like quadratic behaviour with increasing temperature. These results seem to be in qualitative disagreement with the model developed in [8] and [9], where the diagonal approximation [10] for the quasi-particle (QP) excitations spectrum was used, resulting in a quadratic behaviour, $\sim \Delta_0^2$, even at zero temperature.

In [11] and [12] the effect of nonmagnetic impurities on the dHvA oscillations was studied. The authors of [11], solving self-consistently the Green's function equations up to the leading term in Δ_0^2 , found a dramatic enhancement of the damping rate in the SC state with respect to the MS result. They obtained the result that for a Landau level width Γ , satisfying $T \leq \Gamma \ll \hbar\omega_c$, the additional SC induced damping factor, which is the same for all harmonics, is given by:

$$R_s = 1 - \alpha \frac{\pi^{3/2} \Delta_0^2}{\sqrt{n_F}} \tag{1}$$

where $\widetilde{\Delta}_0^2 = \langle \Delta_0^2 \rangle / (\hbar \omega_c)^2 (\langle \ldots \rangle$ means spatial average over vortex lattice), and $\alpha = \frac{1}{2} \left(\frac{\hbar \omega_c}{2\pi\Gamma}\right)^2 \gg 1$. It should be stressed that equation (1), which implies a strong influence of impurity scattering on the dHvA oscillations in the mixed state, is in contrast to the relatively weak thermal effect obtained for pure materials [4, 5] and in contrast also to the results of [12], where the damping associated with impurity scattering turns out to be asymptotically small in the quasi-classical limit $n_F \simeq \mu/\hbar \omega_c \rightarrow \infty$ (μ is a chemical potential): $\alpha = 1 + \alpha_0 \frac{\Gamma}{\omega_c \sqrt{n_F}}$, with $\alpha_0 \sim 1$.

In the present study we examine the impurity scattering effect on the damping of magnetic quantum oscillations near H_{c2} , taking advantage of the Green's function formalism in the quasi-classical limit $\sqrt{n_F} \gg 1$, developed in [5]. This approach, which is based on a direct calculation of the thermodynamic potential, makes it possible to avoid many of the difficulties encountered in [11]. Our results show that in the relaxation time approximation the impurity scattering effect is significantly weaker than that predicted by equation (1), and can be neglected as long as max (πT , Γ) is not too small compared to $\hbar \omega_c$. (For the fundamental harmonic it is found that $\alpha \sim \ln (\hbar \omega_c / \pi \Gamma)$.)

Here we also compare the Gorkov expansion with the thermodynamic potential obtained from the QP spectrum in the diagonal approximation. The agreement between these approaches in the limit of a small broadening of the LLs determines the range of validity of the diagonal approximation and enables us to make new conclusions about the singular nature of the dHvA oscillations in the low-temperature, pure limit, which arises from the infinite degeneracy of the Landau levels. It is also shown that in this limit the diagonal approximation agrees with the numerical calculations made by Norman *et al.*

Restricting our analysis to the close vicinity of the upper critical field H_{c2} , we consider only the leading (i.e. quadratic) term in the Gorkov's expansion of the SC free energy in the order parameter. A 2D electron gas model is used. However, the obtained results for the amplitude of the first harmonic at a given magnitude of the order parameter are valid also for isotropic 3D superconductors, since the main contribution to the oscillating part of the thermodynamic potential comes from extremal orbits with $k_z \approx 0$. The integration over k_z near the stationary point for a system with arbitrary broadening of LLs yields a constant factor in the amplitude and a phase shift of oscillations by $\pi/4$. Similar modifications take place in the normal-phase magnetization, keeping the relative damping rate unchanged [13].

The quadratic term of the Gorkov expansion for the thermodynamic potential can be expressed through Green's function $G_g(\vec{r}_1, \vec{r}_2; \omega)$ and the impurity-dressed pair potential [11] $\Delta(\vec{r}, \omega)$:

$$\Omega^{(2)} = \frac{a_H^2}{V} \int \left| \Delta^2 \left(\overrightarrow{r} \right) \right| d^2 r - \frac{a_H^4}{\beta} \sum_{\omega} \int d^2 r_1 d^2 r_2 \Phi \left(\overrightarrow{r}_1, \overrightarrow{r}_2; \omega \right)$$
(2)

where

$$\Phi\left(\overrightarrow{r}_{1},\overrightarrow{r}_{2};\omega\right)=\Delta\left(\overrightarrow{r}_{1},\omega\right)G_{g}\left(\overrightarrow{r}_{1},\overrightarrow{r}_{2};\omega\right)\Delta^{\star}\left(\overrightarrow{r}_{2},\omega\right)G_{g}\left(\overrightarrow{r}_{1},\overrightarrow{r}_{2};-\omega\right).$$
(3)

In the above equations V is a Bardeen–Cooper–Schrieffer (BCS) interaction constant, and $\beta = 1/T$, $\omega = \pi T (2\nu + 1)$ and $\nu = 0, \pm 1, \ldots$ are Matsubara frequencies. We have used the units where the Plank constant is equal to unity. All spatial variables are measured in the magnetic length units $a_H = \sqrt{\frac{c}{eH}}$.

Using the standard averaging technique [14] (which may not be valid at very low temperatures because of the neglect of coherent electron paths [15, 16]), the isotropic electron

scattering is described by a single parameter, the electronic momentum relaxation time $\tau_{sc} = 1/2\Gamma$. The region where the dHvA oscillations are significant is $\Gamma \leq \omega_c$. Strictly speaking, however, the parameter $2\pi\Gamma/\omega_c$ can be of the order of 1.

We also neglect in our calculation the effect of impurities on the electron pairing $\Delta(\vec{r}, \omega) \approx \Delta(\vec{r})$. The detailed analysis of Green's functions in [11] justifies this approximation. In particular, it was shown there that the correction to the pair potential is small ($\sim 1/\sqrt{n_F} \ll 1$) in the quasi-classical limit under consideration.

The order parameter is selected as a lattice distribution function from the lowest Landau level space [17]. In the symmetric gauge

$$\Delta(x, y) = \left(\frac{2\pi}{a_x^2}\right)^{1/4} \Delta_0 e^{ixy} \sum_n e^{i\gamma n^2 + iq_n x - (y+q_n/2)^2}$$
(4)

where the numbers γ and a_x are arbitrary and $q_n = \frac{2\pi n}{a_x}$. The magnetic field $\vec{H} = (0, 0, H)$ is assumed to be uniform and perpendicular to the conducting *xy*-plane. The concrete choice of the vortex lattice is not important since, as in pure materials [5], the leading (quadratic) term of the thermodynamic potential does not depend on the spatial arrangement of the vortices. This feature reflects the absence of interaction between vortices in the quadratic term of the free energy.

The single electron Green function, in the relaxation time approximation used, is $G_g(\vec{r}_1, \vec{r}_2; \omega) = \exp\left(-\frac{i}{2} [\vec{r}_1, \vec{r}_2]_z\right) \tilde{G}_g(\rho; \omega)$ where $\vec{\rho} = \vec{r}_2 - \vec{r}_1$ and

$$\widetilde{G}_{g}(\rho;\omega) = \frac{1}{2\pi} e^{-\rho^{2}/4} \sum_{n} \frac{L_{n}\left(\rho^{2}/2\right)}{\mathrm{i}\omega + \mathrm{i}\Gamma sign\left(\omega\right) - \omega_{c}\left(n+1/2\right) + \mu}.$$
(5)

In the above expression L_n is the Lagaurre polynomial of the order *n*. The function \widetilde{G}_g differs from the pure limit electron Green function in a magnetic field [19] by the self-energy correction i Γ sign (ω).

Following the procedure developed in [5] and using the Poisson summation formula, we find the Green function $\widetilde{G}_{g}^{(qc)}$ in the quasi-classical approximation $(n_F \gg 1)$. Substituting $\widetilde{G}_{g}^{(qc)}$ and $\Delta(\vec{r})$ into equations (2) and (3) and integrating over the centre of mass coordinates, $\vec{r} = \frac{1}{2}(\vec{r}_2 + \vec{r}_1)$, the thermodynamic potential per unit volume, $\Omega_{sc} = \Omega^{(2)}/\pi a_H^2 N$, is reduced to the known expression obtained for a pure material with the replacement of $|\omega|$ by $|\omega| + \Gamma$:

$$\Omega_s = \left(\frac{\omega_c^2}{V} - \frac{\sqrt{2}}{\beta a_H^2 \sqrt{n_F}} \sum_{\omega \ge 0} q_\omega \gamma_\omega\right) \widetilde{\Delta}_0^2 \tag{6}$$

where $\gamma_{\omega} = \int_0^{\infty} d\rho \exp\left(-\alpha_{\omega}\rho - \frac{1}{2}\rho^2\right)$ with $\alpha_{\omega} = 2\pi \left(|\omega| + \Gamma\right) / \sqrt{\mu\omega_c}$ is the Cooper-pair spatial correlation function. The sharp damping of the integrand at $\rho \ge 1$ reflects the importance of the local electron pair configurations and justifies the neglect of the turning point region $\left(\rho \sim 2\sqrt{2n_F}\right)$ in the quasi-classical Green function.

The quantity q_{ω} , where

$$q_{\omega} = \frac{1}{2} \frac{e^{X_{\omega}}}{\cosh X_{\omega} - \cos\left(2\pi n_F\right)} \tag{7}$$

and where $X_{\omega} = 2\pi (|\omega| + \Gamma) / \omega_c$, is responsible for the quantum magnetic oscillations. In the low temperature limit, $X_{\omega} \ll 1$, it has a singularity $q_{\omega} \simeq \frac{2}{X_{\omega}^2}$ if a Landau level coincides with the Fermi energy. Therefore, at a fixed $\omega \lesssim \Gamma$ the second order correction in Δ is proportional to $\sim \frac{\Delta_0^2}{\sqrt{n_F \Gamma^2}}$. This seems, at a first sight, to reproduce the dependence (equation (1)) found in

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[11]. However, as we shall see below, the summation over Matzubara frequencies leads to a different result.

The Fourier series expansion of q_{ω} is

$$q_{\omega} = a_{\omega}^{(0)} + 2\sum_{k=1}^{\infty} a_{\omega}^{(k)} \cos\left(2\pi k n_{F}\right)$$
(8)

where the coefficient $a_{\omega}^{(k)}$,

$$a_{\omega}^{(k)} = \frac{\exp\left[-2\pi k \left(\Gamma + |\omega|\right) / \omega_{c}\right]}{1 - \exp\left[-4\pi \left(\Gamma + |\omega|\right) / \omega_{c}\right]} \tag{9}$$

determines the damping of the *k*-harmonic. This last expression shows the principal difference between uniform and oscillating parts of the thermodynamic potential. As the dominant contribution to the oscillating part of the thermodynamic potential comes from the energy interval $2\pi |\omega| \leq \omega_c$, the uniform part, as is readily seen from the definition of γ_{ω} , is dominated by the significantly broader energy range $2\pi |\omega| \leq \sqrt{n_F}\omega_c$. In other words, this result means that the oscillating part of the Cooper-pair condensation energy is determined by a few Landau levels near the Fermi surface, whereas for the uniform part about $\sqrt{n_F} \gg 1$ Landau levels contribute.

Using equations (6) and (8) the oscillatory part of the magnetization, $M_s = -\partial \Omega_s / \partial H$, is determined by the strongly oscillating density of states function q_{ω} . It should be noted that in the self-consistent theory, where the order parameter corresponds to a minimum of Ω_s , the oscillations of the order parameter do not influence significantly the magnetization, since the term $\frac{\partial \Omega_s}{\partial \Lambda} \frac{\partial \Lambda}{\partial H}$ is exactly zero. Therefore, the leading harmonic of the magnetization is [18]

$$M_s^{(1)} = -\frac{2\sqrt{\pi}\mu}{\phi_0} \left(\frac{4\pi^2 T}{\omega_c} \sum_{\omega} a_{\omega}^{(1)}\right) \frac{\widetilde{\Delta}_0^2}{\sqrt{n_F}} \sin\left(2\pi n_F\right)$$
(10)

where $\phi_0 = \pi c/e$ is the electronic flux quantum. In deriving this expression it is assumed that $\alpha_{\omega} \ll 1$, so that $\gamma_{\omega} = \sqrt{\pi/2}$. Due to the large values of the filling factor n_F , this condition is usually satisfied even for relatively large temperatures or LL width.

If the impurity broadening or temperature is large, i.e. if $4\pi (\Gamma + \pi T) / \omega_c \gtrsim 1$, then only the first harmonic in equation (8) survives. In this case $a_{\omega}^{(1)} \approx \exp[-2\pi k (\Gamma + |\omega|) / \omega_c]$, so that the scattering by impurities does not influence R_s , which is determined by equation (1) with $\alpha = 1$.

In the low temperature limit the sum over ω may be replaced by an integral. The simple integration leads to

$$\sum_{\omega} a_{\omega}^{(1)} = \frac{\omega_c}{8\pi^2 T} \ln\left[\frac{1 + \exp\left[-2\pi \left(\Gamma + \pi T\right)/\omega_c\right]}{1 - \exp\left[-2\pi \left(\Gamma + \pi T\right)/\omega_c\right]}\right].$$
 (11)

Substituting equation (11) into equation (10), one obtains $\alpha = \frac{1}{2} \ln \left(\frac{\omega_c}{\pi(\Gamma + \pi T)} \right)$ at low impurity density $2\pi \Gamma/\omega_c \ll 1$. At $2\pi \Gamma/\omega_c \gtrsim 1$ we again recover MS-like damping with $\alpha = 1$.

It is well known [20] that if the LLs are narrow the shape of the oscillations deviates significantly from the fundamental harmonic shape; that is, the contributions of higher harmonics become important. We discuss this problem by considering our 2D system in the limit when $\Gamma_{ef} = \max(\Gamma, \pi T) \ll \omega_c$ so that the oscillation pattern has a saw-tooth shape. Excluding from q_{ω} the zero harmonic, the oscillating part of the thermodynamic potential transforms to

$$\Omega_{s,osc} \sim \frac{\widetilde{\Delta}_0^2}{\sqrt{n_F}} \int d\omega \frac{\cos\left(2\pi n_F\right) e^{X_\omega} / \cosh X_\omega}{\cosh X_\omega - \cos\left(2\pi n_F\right)}.$$
(12)

Here the sum over Matsubara frequency is replaced again by an integral. Estimating the maximal value of Ω_{osc} , which is obtained for an integer n_F , we arrive at a simple result

$$\Omega_{s,osc} \sim \frac{\widetilde{\Delta}_0^2}{\sqrt{n_F}} \frac{\omega_c}{\Gamma_{ef}}.$$
(13)

This implies that the damping of the higher harmonics is much stronger in this limit than it is in that of the fundamental one.

It is interesting now to compare the results obtained from the Gorkov expansion with the calculation based on the QP density of states, where the spectrum is given by the diagonal approximation, i.e. $E_n(\vec{q}, k_z) = \sqrt{\varepsilon_n^2(k_z) + \Delta_n^2(\vec{q})}$ where $\varepsilon_n(k_z) = \omega_c(n + \frac{1}{2}) + \frac{k_z^2}{2m} - \mu$, and $\Delta_n(\vec{q})$ is the diagonal matrix element of the (momentum space) pair potential in the Landau levels representation [10]. This is done by generalizing the formalism developed in [20] for a 2D free electron gas to the system of independent QPs described above. The resulting oscillatory part of the thermodynamic potential is given by:

$$\Omega_{osc} = 2D_2 \frac{(m\omega_c)^{1/2}}{\pi} \sum_{p=1}^{\infty} (-1)^p \Theta_p \frac{\cos\left(2\pi pn_F - \pi/4\right)}{\sqrt{p}}$$
(14)

where $D_2 = m/2\pi$ is the 2D single electron density of states, and the integral

$$\Theta_p = \int_0^\infty \frac{\mathrm{d}\omega}{\omega^2} \frac{\pi\omega/\beta}{\sinh\left(\pi\omega/\beta\right)} e^{-\omega\Gamma} \Xi_p\left(\omega\right) \tag{15}$$

is obtained from a product of the Fourier transforms of three distributions: the Fermi distribution function accounting for the finite temperature smearing; the Lorentz distribution arising from the impurity scattering; and $\Xi_p(\omega) = \left(\frac{1}{\pi} \int_{-\infty}^{\infty} d\xi \cos\left(\omega \sqrt{\xi^2 + \Delta_{n_F}^2(\vec{q})}\right) \cos(\tau_p \xi)\right)$, which arises from the scattering by the pair potential. Here $\tau_p = 2\pi p/\omega_c$ and $\langle \ldots \rangle$ stands for integration in \vec{q} space over the magnetic Brillouin zone. It is obvious that for a vanishing order parameter equation (14) reduces to the well known Lifshitz–Kosevich formula. In the general case

$$\Xi_{p}(\omega,q) = \delta\left(\omega - \tau_{p}\right) - \left\langle \frac{J_{1}(x)}{2x} \omega \Delta_{n_{F}}^{2} \right\rangle \theta\left(\omega - \tau_{p}\right)$$
(16)

where $x = \Delta_{n_F} \sqrt{\omega^2 - \tau_p^2}$ and $J_1(x)$ is the Bessel function. The superconducting contribution to the thermodynamic potential is given by the second term on the RHS of equation (16).

Substituting equation (16) into equation (15) one can easily see that the integral over ω diverges logarithmically in the limit $\Gamma_{ef} = \max(\pi T, \Gamma, \Delta) \rightarrow 0$ where $\Delta \sim \sqrt{\langle \Delta_{n_F}^2 \rangle}$. Hence, the maximal characteristic value of ω is limited by $\sim 1/\Gamma_{ef}$. Using $\langle \Delta_{n_F}^2 \rangle = \Delta_0^2/\sqrt{\pi n_F}$ [21] we arrive at the damping rate for the first harmonic in the form

$$R_s = 1 - \ln\left(\frac{\omega_c}{2\pi\Gamma_{ef}}\right) \frac{\pi^{3/2} \tilde{\Delta}_0^2}{\sqrt{n_F}}.$$
(17)

At $\Delta \ll \pi T$ and $\Gamma \ll \omega_c/2\pi$ this expression is consistent with that obtained from the Gorkov expansion. However, with increasing temperature or Γ the results of the two approaches tend to deviate from each other. Such behaviour is caused by a deviation from the diagonal approximation as we move far from the H_{c2} -line.

In the opposite case, when the broadening of LLs due to impurity scattering or the thermal smearing is weak, the influence of the energy levels degeneracy becomes important, leading

to a non-analytical dependence on the pair potential $R_s = 1 - \frac{\pi^{3/2} \widetilde{\Delta}_0^2}{\sqrt{n_F}} \ln\left(\frac{1}{\widetilde{\Delta}_0}\right)$. This result is nothing but the Miyake–Miller–Gyorffy formula in the asymptotic limit $\widetilde{\Delta}_0 \rightarrow 0$. Appearance of the logarithmic term is a reflection of the divergence of the expansion in $\widetilde{\Delta}_0^2$ in the singular limit of the degenerate LLs, $(\pi T, \Gamma) \rightarrow 0$.

Using the above results one can discuss the validity of the Gorkov expansion near H_{c2} . As before, we consider only the oscillating part of the leading term. For a small but finite value of max $(\pi T, \Gamma)$ (i.e. $\ll \omega_c/2\pi$) the SC correction is small provided $\Delta \leq \max(\pi T, \Gamma)$. In this case, equation (6) is a good approximation for Ω_s . With the field decrease (so that $\Delta > \max(\pi T, \Gamma)$) the level broadening is caused mostly by the effect of the order parameter, thus leading to a singular behaviour of Ω_{osc} , which obviously cannot be recovered by a finite number of the Gorkov's expansion terms. It is interesting to note that with a further decrease of the field when the width is comparable with ω_c , i.e. when $2\pi \Delta \sim \omega_c$, we again return to the MS-like damping of the first harmonic.

In the opposite limit, max $(\pi T, \Gamma) \gtrsim \omega_c/2\pi$, which is usually satisfied in experiments, the leading term of the Gorkov expansion, equation (6), describes accurately the thermodynamic potential in the entire range of magnetic fields near H_{c2} , $\Delta \leq \omega_c$. Because the diagonal approximation does not describe correctly the higher order terms in Δ , for which the phase coherence is crucial [2], we do not consider here the low-field limit $\Delta \gtrsim \omega_c$.

Returning to equation (13), one can now estimate the thermodynamic potential when the LL broadening is determined by the pair potential, i.e. when $\Gamma_{ef} \sim \sqrt{\langle \Delta_{n_F}^2 \rangle} \sim \tilde{\Delta}_0/n_F^{1/4}$, so that

$$\Omega_{s,osc} \sim \widetilde{\Delta}_0 / n_F^{1/4}. \tag{18}$$

Such a dependence was extracted from the numerical solution of the Bogoliubov–de Gennes equations by Norman *et al* for a pure 2D SC in the low-temperature region $T/\omega_c \leq 0.04$. It should be stressed that the linear dependence on $\widetilde{\Delta}_0$ is characteristic of a 2D system. In a 3D SC the contribution of the higher harmonics is smaller due to \sqrt{p} in equation (14), which gives rise to $\sim \widetilde{\Delta}_0^{3/2}$ dependence.

In conclusion, we have shown that in the case of narrow Landau levels the SC-induced damping of the magnetic quantum oscillations is governed by the smearing mechanism with the largest characteristic width parameter of all three types of broadening, i.e. impurity scattering, thermal smearing, and the effect of the pair-potential. When the width becomes comparable with the interlevel distance, i.e. when $2\pi \Gamma_{ef}/\omega_c \sim 1$, any dependence of the SC-induced damping factor, R_s , on broadening disappears and to leading order in the SC order parameter R_s is given by equation (1) with $\alpha = 1$. Similar to the magnetic oscillations in the normal-phase the dependence of the fundamental harmonic amplitude on Γ_{ef} turns out to be weaker than of the higher ones.

Finally, it should be stressed that our analysis in this communication is restricted to magnetic oscillations near the upper critical field. Extension of such an analytical approach to the low field region deep in the SC state is a very difficult task. Generally speaking, however, we expect that similar to pure materials [5], the higher order terms in the Gorkov expansion are determined by the expansion parameter $\sim \Delta_0^2/\Gamma_{ef}^2 n_F$ in the case when $\Gamma_{ef} = \max(\pi T, \Gamma) \ll \omega_c/2\pi$ and $\sim \Delta_0^2/\omega_c^2 n_F$ for $\Gamma_{ef} \gtrsim \omega_c/2\pi$. In the low magnetic field limit, when this parameter becomes large, one should sum up all terms of the perturbation series. An example of such a summation in the limit $\Gamma_{ef} \ll \omega_c/2\pi$ and for the most singular case, when a Landau level lies at the Fermi energy, was given in [22]. However, in the general case the behaviour of the thermodynamic potential is unknown. The QP density of state approach also leads to serious difficulties arising from the complex QP spectrum due to

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off-diagonal Landau level pairing [23]. An interesting attempt to consider the low field limit was made in [24], where the spatial variation of $|\Delta|$ was neglected due to the small size of the vortex core region.

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