

## Strong quantum oscillations in the order parameter of two-dimensional type-II superconductors

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(Received 3 June 1991)

Strong magnetic quantum oscillations in the order parameter are predicted to appear at low temperatures in extremely type-II, highly two-dimensional superconductors. The mean-square modulus of the order parameter over the entire vortex lattice near  $H_{c2}(T)$  is calculated using the Gorkov's scheme in the semiclassical approximation. It is found that the strong magnetic quantum oscillations in the order parameter may yield a periodic reentrance of the superconducting state in the vicinity of the upper critical field, smearing greatly the superconducting transition. In systems with critical fields as high as those in the high- $T_c$  cuprates, the fine structure of the oscillations is affected by the pairing correlation. The experimental feasibility of observing quantum oscillations in the highly two-dimensional, high- $T_c$  bismuth compounds is discussed. They are found to persist well below  $H_{c2}(T)$ , indicating the possibility of observing quantum oscillations in the order parameter at experimentally accessible fields.

The discovery of the high- $T_c$  superconductors introduces into the group of layered conductors a new family of superconducting materials, and poses a challenging question concerning possible mechanisms for the high- $T_c$  superconductivity. Since the conventional (BCS) superconductivity is caused by the instability of the Fermi surface (FS), the detailed study of the FS is, obviously, of primary importance in any attempt to sort out these mechanisms. The most powerful methods of studying FS in normal metals are associated with the magnetic quantum oscillations of the thermodynamical and transport properties.

The effect of magnetic quantum oscillations in the superconducting state was considered theoretically by Gunther and Gruenberg<sup>1</sup> and by Ragagopal and Vasudevan.<sup>2</sup> In investigating the layered dichalcogenide  $2H$ -NbSe<sub>2</sub>, Graebner and Robbins<sup>3</sup> observed experimentally significant magnetothermal and dHvA oscillations well below  $H_{c2}$ .

It is well known<sup>4-6</sup> that a strong anisotropy of the FS results in the enhancement of the magnetic quantum oscillations. In a two-dimensional electron gas, the electronic density of states is singular at the Landau levels. The third dimension smears out this singularity, thus strongly reducing the strength of the magnetic quantum oscillations. The highly two-dimensional (2D) character of the relevant electronic properties in some of the high- $T_c$  materials, e.g., the bismuth-based compounds,<sup>7</sup> suggests that magnetic quantum oscillations in the superconducting state could be sufficiently strong to be used as a source of reliable Fermi-surface information.

However, experimental studies of the Fermi surface in this family of materials will not be easy both because the

normal-state resistivity is so large and because the critical temperature and field are so high. The latter disadvantage may turn, however, into a great advantage if the desired quantum oscillations can be observed in the superconducting state, far below  $T_c$ . Our preliminary theoretical analysis shows<sup>8,9</sup> that there is no fundamental obstacle to the coexistence of superconducting order and magnetooscillations in extremely type-II, highly 2D superconductors such as the high- $T_c$  oxides. Furthermore, despite their large normal-state resistivity, some of the high- $T_c$  materials exhibit nearly zero residual resistivity as extrapolated from the high-temperature normal-state data.<sup>10</sup> The large values of the critical parameters,  $T_c$  and  $H_{c2}$ , may now be used to advantage, since they enable one to work at very high magnetic fields (and low temperatures) in order to resolve individual Landau levels, but without destroying the overall superconducting order. The observation of quantum oscillations in the superconducting state would be of great importance not only as a Fermi-surface probe, but also as a way of sorting out the very nature of the yet unknown pairing mechanism in this class of materials.

In this paper we present an analytical expression for the mean-square modulus of the superconducting order parameter at large, quantizing, magnetic fields for a model two-dimensional electron gas in the semiclassical limit (i.e., many occupied Landau levels) corresponding to realistic experimental conditions. Previous attempts to calculate this quantity<sup>11,12</sup> did not take into account the effect of Landau quantization.

We assume a two-dimensional free-electron gas model with a simple BCS pairing interaction under a strong quantizing magnetic field in the vicinity of  $H_{c2}(T)$  for an

arbitrary temperature  $0 < T < T_c$ . For the sake of simplicity, we assume that the effective  $e$ - $e$  interaction  $V$  is independent of the field. Near the critical point, the order parameter  $\Delta(\mathbf{r})$  is small and the superconducting free energy can be expanded to fourth order:

$$F_s = - \int d^2r_1 d^2r_2 \left[ Q(\mathbf{r}_1, \mathbf{r}_2) - \frac{1}{V} \delta(\mathbf{r}_1 - \mathbf{r}_2) \right] \Delta^*(\mathbf{r}_2) \Delta(\mathbf{r}_1) + \int d^2r_1 d^2r_2 d^2r_3 d^2r_4 R(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) \times \Delta(\mathbf{r}_4) \Delta^*(\mathbf{r}_3) \Delta^*(\mathbf{r}_2) \Delta(\mathbf{r}_1), \quad (1)$$

$$Q(\mathbf{r}_1, \mathbf{r}_2) = \frac{k_B T}{\hbar^2} \sum_{\nu=-\infty}^{\infty} G_{\uparrow}^0(\mathbf{r}_2, \mathbf{r}_1; -\omega_{\nu}) G_{\downarrow}^0(\mathbf{r}_2, \mathbf{r}_1; \omega_{\nu}), \quad (2)$$

$$R(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) = \frac{k_B T}{\hbar^4} \sum_{\nu=-\infty}^{\infty} G_{\uparrow}^0(\mathbf{r}_2, \mathbf{r}_1; -\omega_{\nu}) G_{\downarrow}^0(\mathbf{r}_2, \mathbf{r}_4; \omega_{\nu}) \times G_{\uparrow}^0(\mathbf{r}_3, \mathbf{r}_4; -\omega_{\nu}) \times G_{\downarrow}^0(\mathbf{r}_3, \mathbf{r}_1; \omega_{\nu}). \quad (3)$$

In the above equations  $G_{\sigma}^0(\mathbf{r}, \mathbf{r}'; \omega_{\nu})$  is the free-electron thermal Green's function with spin  $\sigma$  in the presence of a magnetic field  $\mathbf{H}$  oriented perpendicular to the layers (along the  $z$  axis) and  $\omega_{\nu} = (2\nu + 1)\pi k_B T / \hbar$ ,  $\nu = 0, \pm 1, \pm 2, \dots$ , the thermal Matsubara frequencies. Note that the kernels  $Q$  and  $R$  vary on the length scale of the thermal mean free path  $\xi = \hbar v_F / \pi k_B T$ , while  $\Delta(\mathbf{r})$  varies on the magnetic length scale  $a_H = (c\hbar / eH)^{1/2}$ . For high magnetic fields (and low temperatures),  $\xi > a_H$  and the nonlocal character of the kernels prohibits the use of the gradient expansion, which simplifies greatly the analysis near  $T_c$ .<sup>13</sup> Semiclassical conditions,  $E_F \gg \hbar\omega_c$ , with  $\omega_c = eH / (m_e c)$ ,  $m_e$  the in-plane cyclotron-resonance mass, are still assumed, however, so that using the Landau gauge  $\mathbf{A} = (0, Hx, 0)$  wave functions:

$$\Psi_{n, k_y}(x, y) = e^{ik_y y} \phi_n(x - x_0)$$

with  $x_0 = a_H^2 k_y$ , and the WKB approximation for  $\phi_n(x - x_0)$ :

$$[\phi_n(x - x_0)]_{n \gg 1} \simeq \left[ \frac{2}{\pi a_H} \right]^{1/2} (2n - \xi^2)^{-1/4} \cos[s_n(\xi)], \quad (4)$$

where  $\xi = (x - x_0) / a_H$  and

$$s_n(\xi) = \frac{1}{2} \xi (2n - \xi^2)^{1/2} + n \arcsin(\xi / \sqrt{2n}) - \pi n / 2,$$

the calculation of  $G_{\sigma}^0(\mathbf{r}_1, \mathbf{r}_2; \omega_{\nu})$  is significantly simplified. Here the integral over  $k_y(x_0)$  is performed by the stationary phase method, which is consistent with the semiclassical (WKB) approximation.

The picture of pairing which emerges from this semiclassical analysis is as follows (Fig.1): Any two paired electrons occupy large cyclotron orbits with centers  $x_0, x'_0$  separated by a distance  $|x'_0 - x_0|$  of about  $2a_H \sqrt{2n_0}$ ,  $n_0 \equiv E_F / \hbar\omega_c \gg 1$ . They remain coherent (i.e., satisfy  $k'_y \simeq -k_y$ ) within a distance  $\rho \equiv |\mathbf{r}_1 - \mathbf{r}_2|$  not larger than the magnetic length  $a_H$ . Outside this coher-

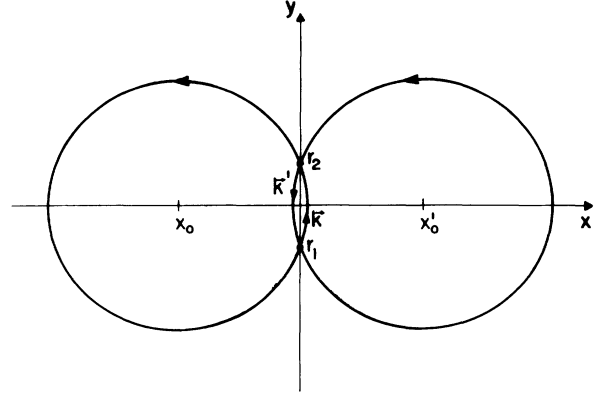


FIG. 1. The semiclassical picture of pairing in a 2D electron gas under a magnetic field. The paired electrons occupy large cyclotron orbits with centers at  $x'_0, x_0$  separated by a distance  $|x'_0 - x_0|$  of about twice the cyclotron radius of the Fermi cylinder, i.e.,  $2k_F a_H^2$ . They remain coherent (i.e., satisfy  $k'_y \simeq -k_y$ ) within a small distance  $|\mathbf{r}_2 - \mathbf{r}_1| \leq a_H$ .

ence length, the contributions to the free energy decay exponentially with  $\rho^2$  [see Eqs. (12) and (13)]. It is therefore sufficient to know the form of the single-electron Green's function appearing in Eqs. (2) and (3) for  $\rho \leq a_H$ , which satisfy  $|\mathbf{r}_1 - \mathbf{r}_2|^2 \ll 8n_0 a_H^2$  in the semiclassical limit (i.e.,  $n_0 \gg 1$ ). Using the Poisson rule for the sum over the Landau levels, this leads to the following result:

$$G_{\sigma}^0(\mathbf{r}_2, \mathbf{r}_1, \omega_{\nu}) = \frac{im_c}{\sqrt{2\pi(2n_0)^{1/2}}} \exp(-ie \mathbf{A} \boldsymbol{\rho} / c\hbar) g_{\sigma}(\rho, \omega_{\nu}) \mathcal{J}_{\sigma}(\omega_{\nu}), \quad (5)$$

where

$$g_{\sigma}(\rho, \omega_{\nu}) = \sqrt{a_H / \rho} \exp \left[ i(\sqrt{2n_0} \rho / a_H) \text{sgn}(\omega_{\nu}) - (|\omega_{\nu}| / 2\omega_c \sqrt{2n_0} \sigma) \left( \frac{\rho}{a_H} \right) \right] \quad (6)$$

and

$$\mathcal{J}_{\sigma}(\omega_{\nu}) = 1 / \left[ 1 - \exp \left[ 2\pi i n_0^{\sigma} \text{sgn}(\omega_{\nu}) - \frac{2\pi |\omega_{\nu}|}{\omega_c} \right] \right], \quad (7)$$

where  $\boldsymbol{\rho} \equiv \mathbf{r}_1 - \mathbf{r}_2$ ,  $n_0^{\sigma} = n_0 - \frac{1}{2} + (\omega_e / \omega_c) \sigma / 2$ ,  $\omega_e = eH / cm_0$  with  $m_0$  the free-electron mass, and  $\mathbf{A}$  is the vector potential at the position  $\frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$ . Note that, in the semiclassical limit,  $\sqrt{2n_0} \sigma = \sqrt{2n_0} + \mathcal{O}(1/\sqrt{2n_0})$ . Thus, the only important dependence on the electron spin in this limit is through  $n_0^{\sigma}$  appearing in the denominator of Eq. (7). With this expression for the Green's function, the kernels  $Q(\mathbf{r}_1, \mathbf{r}_2)$  and  $R(\mathbf{r}_1, \dots, \mathbf{r}_4)$  are readily obtained.

It should be noted here that in a 2D electron gas under a strong magnetic field,  $E_F$  is not field independent.<sup>4-6</sup>

The influence of this effect on the magnetization and on the spin relaxation in high magnetic fields has been studied in detail in Refs. 5 and 6. In real 2D systems, however, the strong oscillations of the chemical potential are severely damped as a result of various, material-dependent, factors.<sup>14</sup> We shall not dwell on this subject here, and in what follows we assume  $E_F = \text{const}(H)$ .

A general variational form for  $\Delta(\mathbf{r})$  in the symmetric gauge, which is restricted only by the assumption that the condensate of Cooper pairs is in the ground Landau level, can be written as<sup>15,16</sup>

$$\Delta(\mathbf{r}) = \Delta_0 \exp\left(-\frac{1}{2}z z^* + \frac{1}{2}z^2\right) g(z), \quad (8)$$

where  $z \equiv (x + iy)/a_H$ , and  $g(z)$  an arbitrary entire function in the complex plane. Specifically, we write  $g(z)$  as a Fourier sum:<sup>16</sup>  $g(z) = \sum_{n=-\infty}^{\infty} c_n e^{2\pi i n z/a_x}$ , where  $a_x$  is an arbitrary constant and  $c_n$  are variational parameters. Using this variational form and the symmetric gauge expressions of the kernels  $Q$  and  $R$  in Eq. (1), the multiple integrals associated with both the quadratic and the quartic terms can be performed analytically.<sup>16</sup> Applying the variational principle to the free energy  $F_s\{c_n\}$ , we get a set of nonlinear equations, which is solved exactly by the array  $c_n$  corresponding to a periodic vortex lattice, provided that the amplitude  $\Delta_0$  satisfies the algebraic equation<sup>16</sup>

$$\Delta_0^2 = \frac{(\pi k_B T_c)^2}{2B} (A - 1/\lambda), \quad (9)$$

where

$$A = 2 \left[ \frac{a_H}{\xi} \right] \sum_{\nu=0}^{\nu_D-1} \text{Re}(q_\nu) \gamma_\nu \quad (10)$$

is the lowest eigenvalue of the linearized gap equation,<sup>1</sup> and  $B$  is associated with the quartic term. We have found that,<sup>16</sup> to a very good approximation,  $B$  can be written as

$$B = \beta_A \left[ \frac{a_H}{\xi} \right] \left[ \frac{a_H}{\xi_0} \right]^{2\nu_D-1} \sum_{\nu=0}^{\nu_D-1} \text{Re}(q_\nu^2) \delta_\nu, \quad (11)$$

where  $\beta_A$  is the well-known geometrical factor<sup>17</sup> of the Abrikosov lattice and the rest depends only on the normal electron properties. In the above equations

$$\gamma_\nu = \int_0^\infty e^{-\alpha_\nu \rho - (1/2)\rho^2}, \quad (12)$$

$$\delta_\nu = 2\pi \int_0^\infty e^{-2\alpha_\nu \rho - \rho^2} [\text{erf}(\rho/\sqrt{2})]^2 d\rho, \quad (13)$$

$$q_\nu = \frac{\exp(2\pi\omega_\nu/\omega_c - i\pi\omega_e/\omega_c)}{[\cosh(2\pi\omega_\nu/\omega_c - i\pi\omega_e/\omega_c) + \cos(2\pi E_F/\hbar\omega_c)]}, \quad (14)$$

where  $\alpha_\nu = 2(2\nu+1)a_H/\xi$  and  $\lambda = N(0)V$  is the effective BCS coupling constant with  $N(0) = m_c/2\pi\hbar^2$  the 2D density of states of the electron gas,  $T_c = 1.134(\pi T_D)e^{-1/\lambda}$ , the zero-field transition temperature,  $\xi = \hbar v_F/\pi k_B T_c$ , the zero-temperature coherence length,  $T_D$  is the cutoff temperature,  $\nu_D = T_D/2T$ , and  $\hbar\omega_e = eH/m_0c$  is the Zeeman splitting of a Landau level. Note that our imaginary

(Matsubara) frequency formalism is equivalent to the real frequency one only at discrete values of the temperature  $T$  for which  $\nu_D$  is an exact integer. We therefore restrict the temperature in our calculation to these values. The zero-field limit of  $A$  and  $B$  in Eqs. (10) and (11) is obtained where  $\alpha_\nu \gg 1$ , i.e., where  $a_H/\xi \gg 1$ . In this limit  $A \rightarrow \sum_{\nu=0}^{\nu_D-1} 1/(\nu+1/2)$ ,  $B \rightarrow \frac{1}{16} \sum_{\nu=0}^{\infty} 1/(\nu+1/2)^3$ , the well-known results near  $T_c$ .<sup>13</sup>

It can be readily shown that

$$\Delta_0^2(H, T) = \frac{1}{\pi N a_H^2} \int d^2r |\Delta(\mathbf{r})|^2,$$

where  $N$  is the total number of vortex lines threading the superconductor. Thus, Eq. (9) provides an explicit expression for the square modulus of the order parameter averaged over the entire Abrikosov lattice. Figure 2 shows numerical results for  $\Delta_0^2(H, T)$  in the range of the relevant parameters, which may characterize the  $\text{Bi}_2\text{CaSr}_2\text{Cu}_2\text{O}_{8+x}$  phase of the Bi-containing superconductors,<sup>7</sup> if the weak-coupling BCS theory is assumed to

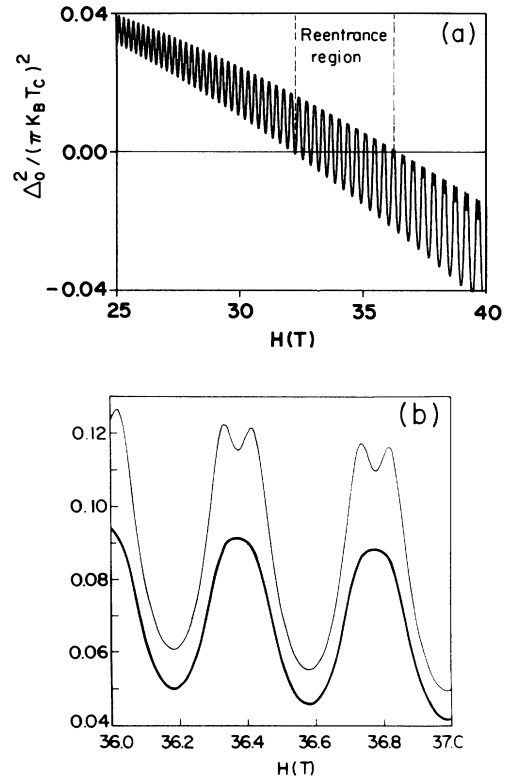


FIG. 2. (a) The mean-square modulus,  $\Delta_0^2$ , of the superconducting order parameter as a function of the magnetic field  $H$  near  $H_{c2}(T)$  for  $T=1$  K. Superconductivity disappears in regions where  $\Delta_0^2 < 0$ . The selected values of the parameters used are  $E_F = 2029$  K,  $m_c = 2.22m_0$ ,  $T_D = 977$  K, and  $T_c = 87$  K. Note, that spin splitting starts being visible above 40 T. (b) The condensation energy  $(A - 1/\lambda)$  [see Eq. (10)] (thin curve) and  $\Delta_0^2$  (thick curve) as functions of  $H$  in a small window between 36 and 37 T, illustrating how the pair-breaking effect due to spin polarization can be quenched by a feedback effect in the pair-pair repulsion.

be valid for this material. The selected values of the parameters are  $T_c = 87$  K,  $E_F = 2029$  K;  $m_c = 2.22m_0$  and  $T_D = 977$  K. The value of the coherence length at  $T = 0$  obtained from these values is  $\xi_0 = 26.4$  Å, which is a reasonable number for the in-plane coherence length. Figure 2 shows that, at low temperatures (1 K), the magnetooscillations in  $\Delta_0^2$  near  $H_{c2}(T)$  are quite strong and remain considerable well below  $H_{c2}$ . The large oscillations in  $\Delta_0^2$  around  $H_{c2}$  lead to periodic disappearance and reentrance of superconductivity with  $1/H$ .

The fine structure of the oscillations, if observable, contain not only Fermi-surface information, but more direct information, concerning the pairing correlation itself. To illustrate the potential significance of this fine structure, we consider a couple of oscillations in the field range  $H = 36\text{--}37$  T (Fig. 2). One expects that Zeeman splitting will show up if the ratio  $m_c/m_0$  is not an integer. Here, however, our result for  $\Delta_0^2(H, T)$  does not show any Zeeman spin splitting of the main dHvA peaks, although the ratio  $m_c/m_0 = 2.22$  is not an integer. The reason for the absence of this splitting becomes clear after considering separately the numerator  $A - 1/\lambda$  and the denominator  $B$  in Eq. (10): In contrast to  $\Delta_0^2$ , the peaks of both  $A$  and  $B$  in this field range are spin split, so that the dips appearing in the peaks of  $B$  tend to cancel the dips appearing in the peaks of  $A$ . Thus, the pair-breaking effect associated with the spin polarization in the magnetic field can be reduced, or even disappear completely, since the feedback of this pair breaking on the pair-pair repulsion tends to lower the superconducting free energy.

Obviously, impurity effects will act to wash the oscillations out. This will take place by smearing the oscillating factor  $q_v$  in much the same way as in an ordinary dHvA effect.<sup>4,5,16</sup>

To summarize, we have shown that the mean-square order parameter for an extremely type-II superconducting state of a 2D electron gas in the clean limit is a strongly oscillating function of the magnetic field near  $H_{c2}(T)$  at low temperatures. These oscillations are found to persist at fields well below  $H_{c2}$  and may lead to a periodic reentrance of the superconducting state well above  $H_{c2}$ .<sup>15,18,19</sup>

It should be noted that a detailed application of our theory to systems with short coherence lengths, such as the high- $T_c$  oxides, must address the effect of fluctuations in the order parameter. As far as the amplitude  $\Delta_0$  is concerned, however, the effect of fluctuations is expected to diminish considerably at low temperatures (and high fields) far below  $T_c$ . The subject of fluctuations of vortex lines is clearly beyond the scope of the present paper. However, the remarkable decoupling found between the oscillatory part of  $B$ , which reflects the behavior of the normal electrons near the Fermi surface, and the part associated with the flux lattice, may indicate that flux lines motion should not affect the oscillations in  $\Delta_0^2$ .

*Note added in proof.* It should be noted that the authors in Refs. 18 expressed strong doubts concerning the reality of reentrant superconductivity as presented in Ref. 15. In Ref. 19 we showed that the likelihood of such a reentrance phenomenon is greatly enhanced in highly 2D systems.

We acknowledge valuable discussions with L. Bulaevskii, W. Joss, D. Shoenberg, Z. Tesanovic, and S. Vedenev. This research was supported by a grant from the German-Israeli Foundation for Scientific Research and Development, No. G-112-279.7/88.

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