de Haas–van Alphen effect in the superconducting state of a two-dimensional metal

T. Maniv
Department of Chemistry and Solid State Institute, Technion-Israel Institute of Technology, Haifa 32000, Israel and Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, Maryland 21218

A. I. Rom
Department of Chemistry, Technion-Israel Institute of Technology, Haifa 32000, Israel

I. D. Vagner
Solid State Institute, Technion–Israel Institute of Technology, Haifa 32000, Israel and Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, Maryland 21218

P. Wyder
Max-Planck-Institut für Festkörperforschung, Hochfeld-Magnetlabor, Boîte Postale 166, F-38042, Grenoble Cedex 9, France

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We present a theory of the de Haas–van Alphen (dHvA) effect in the superconducting mixed state within the framework of Gorkov's scheme near H_{c2} in a two-dimensional (2D), extremely type-II superconductor. A semiclassical approximation is developed whose results are compared to the exact quantum-mechanical result. A remarkable agreement between the two methods is found even for extremely strong fields and low temperatures, where strong quantum oscillations exist. The method is used to calculate variationally the superconducting free energy to the fourth order in the Gorkov expansion. The resulting variational equation for the order parameter is solved exactly, and the mean-square order parameter over the entire vortex lattice, as well as the superconducting magnetization, is calculated as functions of the magnetic field and the temperature. It is found that, despite significant smearing effects of the collective pairing process which involves many Landau levels, strong quantum oscillations exist in the superconducting order parameter. The calculated superconducting magnetization oscillations are of the same order of magnitude as the normal-electron ones. The envelope of these oscillations is found to decay exponentially with increasing magnetic field. At sufficiently low temperatures the fine structure of the oscillations may reflect the repulsive nature of the interaction between vortex lines. The transition to superconductivity is investigated along, and above, the classical Ginzburg-Landau phase boundary: Reentrance of the superconducting state above $H_{c2}(T)$, a dramatic manifestation of the 2D dHvA effect, is found to occur within an experimentally accessible range of fields and temperatures if the cyclotron-effective mass is an integral multiple of the free-electron mass.

I. INTRODUCTION

The behavior of type-II superconductors under very high magnetic fields has become a subject of considerable interest recently,[1–5] especially in the light of reports[6,7] of the observation of de Haas–van Alphen (dHvA) oscillations in 1:2:3 oxide superconductors. The dHvA effect, which is an extremely effective method for investigating Fermi surfaces, may shed light on the highly debated issue concerning the nature of the normal state above the transition to superconductivity.[8] The very existence of well-defined magnetic oscillations seems to imply that a sharp Fermi surface exists for the underlying normal state.

Beyond this direction of research, which is of obvious importance, there is a much less obvious, but presumably not less important line of research: A study of magnetic quantum oscillations *in the superconducting state* near the upper critical field.[2,1] Such a study was carried out more than a decade ago by Graebner and Robbins[9] on the layered transition metal dichalcogenide $2H$-$NbSe_2$. Earlier attempts to investigate this matter were made theoretically by Rajagopal and Vasudevan,[10] and by Gunther and Greunberg,[11] who considered the effect of Landau quantization on the linearized Gorkov equation. They have found that $T_{c2}(H)$ should be an oscillatory function of H and that the period of these oscillations should be the same as that of the normal dHvA oscillations.

The discovery of the oxide superconductors creates a very exciting situation since in these materials working in the superconducting state does not necessarily exclude the use of high magnetic fields.[1,2] Thus the unique combination of extremely type-II character and highly two-dimensional (2D) electronic properties offered by these materials (especially the Bi-based compounds) makes it possible to observe the effect of Landau quantization on the superconducting order parameter.[1,12,13] This may provide valuable information about the very nature of the superconducting state in this class of materials.

Another exciting line of research is the search for new

superconducting ground states in very high magnetic fields, far above the classical Ginzburg-Landau phase boundary. The possibility of superconductivity under very high magnetic fields was indicated soon after the development of Gorkov's semiclassical theory for H_{c2}:[14] Gruenberg and Gunther[11] noted that at zero temperature H_{c2} could be arbitrarily large, provided that impurity scattering and Zeeman spin splitting are ignored. Recently Tešanovic, Rasolt, and Xing[3] considered the extreme quantum limit in an isotropic 3D system, when only the ground electronic Landau level is occupied, and found a reentrant superconducting state far above the classical Ginzburg-Landau phase boundary. This may be realized in low density electron gas systems, such as doped semiconductors. The issue was considered by other authors,[15,16] who reexamined the linearized Gorkov equation in great detail, and expressed some doubts concerning the reality of this effect.

Stimulated by these developments, several authors[4,5,17] have extended the discussion to the vortex state far away from H_{c2}, by considering the Bogoliubov–de Gennes equations[18] in the limit when a small number of Landau levels are occupied. This is of fundamental interest since it is concerned with quasiparticle excitations in a 2D system in the limit when charged particles and vortices interact strongly.[19,20]

The aspect which makes the superconducting state so unusual and exciting at a high magnetic field is the enhancement of the single-electron density of states in certain field regions. Cooper pairing in these regions is reinforced and this may compete with the destructive nature of the magnetic field with respect to the superconducting order. In a 2D electron system the density of states is singularly enhanced at the Landau levels, while the introduction of the third dimension smears out this singularity. It is therefore of great interest to investigate the effect of magnetic quantum oscillations in the superconducting state of an ideal, two-dimensional, model system in the extremely type-II case, which is actually the case in some high-T_c oxides.

In this paper we provide a detailed exposition of our theory of Landau quantization in the superconducting state of a 2D electron gas.

We use the standard Gorkov scheme for the expansion of the superconducting free energy in a nonuniform order parameter, and apply a semiclassical approximation to the single-electron Green's functions: We take advantage of the large difference in length scales between the cyclotron radius of electrons at the Fermi energy and that of Cooper pairs in the ground Landau level (the coherence length) for the semiclassical situation considered, and find a simple expansion for the single-electron Green's functions, which enter into the pairing correlation functions. This enables us to calculate analytically not only the quadratic term in the free energy in Gorkov's scheme, but also the quartic term. Our approximation is carefully tested versus the exact quantum-mechanical result, available for the quadratic term. Excellent agreement is found even in cases when the semiclassical scheme is expected to break down. The resulting free energy is written in a variational form similar to that of Abrikosov. The corresponding equations for the variational coefficients are a generalized version of the Abrikosov variational equations.[21] They are solved explicitly and the resulting coefficients are found to satisfy the Abrikosov recursion relations. All these enable us to compute the mean-square order parameter over the entire vortex lattice, as well as any physical quantity which is a functional of the order parameter.

In addition to the complete formal presentation we exhibit results of an extensive numerical study, which includes quantum oscillations in the order parameter and in the magnetization associated with both the superconducting and the normal electrons. Our main concern here is in identifying and analyzing structures in the dHvA effect which are unique to the superconducting state, and can be measured experimentally.

II. PAIRING IN A 2D ELECTRON GAS UNDER A MAGNETIC FIELD

A. General representation

We consider a pure, 2D electron gas (in the $x-y$ plane) under a perpendicular magnetic field H (along the z axis). The Landau-gauge free-electron Green's function with spin σ is given by

$$G_\sigma^0(\mathbf{r}_2,\mathbf{r}_1;\omega_\nu)=\frac{1}{L_y}\sum_{k_y} e^{ik_y(y_2-y_1)}\sum_n \frac{\phi_n(x_1-x_0)\phi_n(x_2-x_0)}{i\omega_\nu-\omega_c(n+\frac{1}{2})-\omega_e\sigma/2+\mu}\ , \tag{1}$$

where $\phi_n(x-x_0)$ is the one-dimensional harmonic-oscillator wave function with energy $\hbar\omega_c(n+\frac{1}{2})$, centered at $x_0=k_y a_H^2$, with $a_H^2=c\hbar/eH$; $\omega_\nu=(2\nu+1)\pi k_B T/\hbar$, $\nu=0,\pm1,\ldots$, are the thermal Matsubara frequencies; $\omega_c=eH/m_c c$ is the cyclotron frequency; $\omega_e=eH/m_0 c$, with m_0 the free-electron mass, is the Zeeman frequency; and $E_F=\hbar\mu$ is the Fermi energy.

For the sake of simplicity we assume a simple BCS pairing interaction V which is independent of the magnetic field. Near the upper critical field $H_{c2}(T)$ at an arbitrary temperature $0<T<T_c$, the order parameter $\Delta(\mathbf{r})$ is small and the superconducting free energy can be expanded in $\Delta(\mathbf{r})$. To fourth order, one has

$$F_s=F_s^{(2)}+F_s^{(4)}\ , \tag{2}$$

where

$$F_s^{(2)}=\int d^2r_1\int d^2r_2\left[\frac{1}{V}\delta(\mathbf{r}_1-\mathbf{r}_2)-Q(\mathbf{r}_1,\mathbf{r}_2)\right]\times\Delta^*(\mathbf{r}_2)\Delta(\mathbf{r}_1) \tag{3}$$

and

$$F_s^{(4)}=\int d^2r_1\int d^2r_2\int d^2r_3\int d^2r_4 R(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4)\times\Delta(\mathbf{r}_4)\Delta^*(\mathbf{r}_3)\times\Delta^*(\mathbf{r}_2)\Delta(\mathbf{r}_1)\ , \tag{4}$$

where the kernel $Q(\mathbf{r}_1,\mathbf{r}_2)$ is given by

$$Q(\mathbf{r}_1,\mathbf{r}_2)=\frac{k_BT}{\hbar^2}\sum_{\nu=-\infty}^{\infty}G_\sigma^0(\mathbf{r}_2,\mathbf{r}_1;\omega_\nu)G_{-\sigma}^0(\mathbf{r}_2,\mathbf{r}_1;-\omega_\nu) \tag{5}$$

and

$$R(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4)=\frac{k_BT}{\hbar^4}\sum_{\nu=-\infty}^{\infty}G_\sigma^0(\mathbf{r}_2,\mathbf{r}_1;-\omega_\nu)\times G_{-\sigma}^0(\mathbf{r}_2,\mathbf{r}_4;\omega_\nu)\times G_\sigma^0(\mathbf{r}_3,\mathbf{r}_4;-\omega_\nu)\times G_{-\sigma}^0(\mathbf{r}_3,\mathbf{r}_1;\omega_\nu)\ . \tag{6}$$

To investigate the pairing instability we consider the linearized Gorkov equation for the pair potential $\Delta(\mathbf{r})$:

$$\int d^2r_2 Q(\mathbf{r}_1,\mathbf{r}_2)\Delta^*(\mathbf{r}_2)=\frac{1}{V}\Delta^*(\mathbf{r}_1)\ . \tag{7}$$

The integral operator Q has a infinitely degenerate manifold of eigenfunctions, which can be represented as[3]

$$\Delta(x,y)=\Delta_0 e^{-(1/2)zz^*}f(z)\ , \tag{8}$$

where $z=(x+iy)/a_H$ and $f(z)$ is an arbitrary entire function in the complex plane. This form corresponds to the symmetric gauge, where the vector potential is given by $\mathbf{A}(\mathbf{r})=\frac{1}{2}\mathbf{r}\times\mathbf{H}$. The corresponding eigenvalue has been calculated by Rajagopol and Vasudevan[10] for a 3D electron gas. In our 2D system it takes the form

$$A=\tfrac{1}{2}\hbar\omega_c\sum_{n,n'=0}^{\infty}\frac{(n+n')!}{n!n'!2^{n+n'}}k_BT\times\sum_\nu g_{n,\sigma}(i\omega_\nu)g_{n',-\sigma}(-i\omega_\nu)\ , \tag{9}$$

with

$$g_{n,\sigma}(i\omega_\nu)=\frac{1}{[i\omega_\nu-\omega_c(n+\frac{1}{2})+\mu-\frac{1}{2}\omega_e\sigma]\hbar}\ . \tag{10}$$

Note that this triple sum is divergent. A cutoff should be introduced either by truncating the Matsubara sum at $\nu=\nu_D-1$, with $\nu_D=\frac{1}{2}(T_D/T)$, and where T_D is the effective "Debye" temperature, or by restricting $n+n'$ to lie between $2n_0-n_D$ and $2n_0+n_D$, with $n_D=\pi k_BT_D/\hbar\omega_c$. The latter procedure leads to the following expression:

$$A=\tfrac{1}{2}\sum_{n,n'=0;n+n'=2n_0-n_D}^{n+n'=2n_0+n_D}\frac{(n+n')!}{n!n'!2^{n+n'}}\frac{\tanh(\beta\varepsilon_n/2)+\tanh(\beta\varepsilon_{n'}/2)}{n+n'+1-2n_F}\ , \tag{11}$$

where $\varepsilon_n/\hbar=(n+\frac{1}{2})\omega_c-\mu-\frac{1}{2}\omega_e$, $\varepsilon_{n'}/\hbar=(n'+\frac{1}{2})\omega_c-\mu+\frac{1}{2}\omega_e$, and $\beta=1/k_BT$. It should be emphasized that the two procedures do not yield exactly the same result. It is clear that the procedure which leads to Eq. (11) is the more physical way of introducing the cutoff, since it applied to real energies. We shall discuss this issue later in Sec. IV.

Note that Eq. (11), without the combinatorial factors, and after restricting the sums over the Landau levels to diagonal terms ($n'=n$) only, is identical to half of the BCS expression for the condensation energy. In the low-field limit, however, the full expression (11) tends to the BCS result. Thus the off-diagonal terms are as important as the diagonal ones in this limit. This property remains valid even at large fields, provided that the number of occupied Landau levels is large.[22]

The eigenvalue A corresponds to the ground Landau orbital of the entire condensate of Cooper pairs in the magnetic field. The arbitrariness of the function $f(z)$ thus reflects the degeneracy of this ground state in the limit where the nonlinear terms in the Gorkov expansion are neglected. The zeros of $f(z)$ in the complex plane are the points where the magnetic flux lines thread in 2D superconductor. Thus the arbitrariness of the location of the zeros reflects the absence of any interaction between vortex lines in this state.

The degeneracy is, however, removed by the nonlinear terms, which introduce effective interaction between the vortex lines. As we shall see later, the solutions of the nonlinear equation in arbitrary magnetic field correspond to periodic (Abrikosov) vortex lattices, as in the classical Ginzburg-Landau (low-field) limit. For an extremely type-II superconductor the resulting close-packed vortex lattice corresponds to a lattice of highly overlapping flux tubes. Thus the electrons in our 2D system are affected by a strong, uniform magnetic field, which forces them into well-defined cyclotron orbits, provided that the effect of scattering by impurities is sufficiently small. This leads, at sufficiently low temperatures, to strong quantum oscillations in the eigenvalue A as a function of H.

B. The semiclassical picture of pairing

To gain insight into the phenomenon of pairing in our 2D system under a magnetic field it is quite necessary to make some approximations. The semiclassical approximation is found quite useful in this regard, and usually it is very well justified, even for very large magnetic fields.

In the semiclassical limit, $n_F=E_F/\hbar\omega_c\gg1$, one may invoke the WKB approximation of the wave functions $\phi_n(x-x_0)$ and use the stationary phase approximation to calculate the Green's function in Eq. (1). In this approach the interpretation of the phase integral leads to a clear classical picture of the pairing orbits.

Thus in the WKB approximation one has

$$\phi_n(x-x_0)=\left[\frac{2}{\pi a_H}\right]^{1/2}(2n-\xi^2)^{-1/4} \times \cos[S_n(\xi)], \quad n\gg 1 , \tag{12}$$

where

$$S_n(\xi)=\tfrac{1}{2}\xi(2n-\xi^2)^{1/2}+n\arcsin(\xi/\sqrt{2n})-\pi n/2 \tag{13}$$

and $\xi=(x-x_0)/a_H$. Transforming the sum over k_y in Eq. (1) to an integral over x_0, and performing the integral by the stationary phase method, which is consistent with the semiclassical approximation used, the equation for the stationary point can be written in the form

$$\left[x_0-\frac{x_1+x_2}{2}\right]^2=\tfrac{1}{2}(y_1-y_2)^2(8na_H^2/\rho^2-1) , \tag{14}$$

where $\rho^2=(x_1-x_2)^2+(y_1-y_2)^2$. As we shall see later, propagation distances ρ that are much larger than the magnetic length a_H contribute very little to the pair correlation function $Q(\mathbf{r}_1,\mathbf{r}_2)$. Thus, since in the semiclassical limit $n\gg 1$, we may assume that $\rho^2\ll 8na_H^2$ in Eq. (14) and find, for the stationary point,

$$x_0\approx\tfrac{1}{2}(x_1+x_2)\pm\sqrt{2n}\,a_H\frac{y_1-y_2}{\rho} . \tag{15}$$

Expanding the Green's function in the small quantity $(\rho/\sqrt{8n}\,a_H)^2$ we find that, to leading order,

$$G_\sigma^0(\mathbf{r}_2,\mathbf{r}_1;\omega_\nu)=-\sum_{n'=-n_0}^{\infty}\frac{g^\nu_{n'+n_0}(\mathbf{r}_2,\mathbf{r}_1)}{n'-\mu_\sigma^F-i\omega_\nu/\omega_c} , \tag{16}$$

where

$$g_n^\nu(\mathbf{r}_2,\mathbf{r}_1)=(2\pi a_H)^{-3/2}(2n\rho)^{-1/2} \times\exp\left[-\frac{ie}{\hbar c}\mathbf{A}\cdot\boldsymbol{\rho}+i(2n)^{1/2}\operatorname{sgn}(\omega_\nu)\frac{\rho}{a_H}\right] , \tag{17}$$

$\mathbf{A}$ is the vector potential at the mean position $\frac{1}{2}(\mathbf{r}_1+\mathbf{r}_2)$, and

$$\mu_\sigma^F=n_F-n_0-\tfrac{1}{2}-\frac{m_c}{2m_0}\sigma . \tag{18}$$

Here n_0 is defined as the integral value of $n_F\equiv E_F/\hbar\omega_c$.

This expression can be further simplified if the lower limit, $-n_0$, of the sum over n' in Eq. (16) is replaced by $-\infty$. Moreover, since the energy denominator in Eq. (16) is minimal at $n'\equiv n-n_0=0$, or ± 1, and as long as $E_F\gg k_BT$, we may also approximate the quantity $(2n)^{1/2}$ in Eq. (17) by $(2n)^{1/2}=(2n_0)^{1/2}+n'/(2n_0)^{1/2}+\cdots$. Using the Poisson summation formula for the sum over n' and performing the integration by the residue method, we find that

$$G_\sigma^0(\mathbf{r}_2,\mathbf{r}_1;\omega_\nu)=-\frac{1}{\omega_c(2\pi a_H)^{3/2}(2n_0)^{1/4}}\rho^{-1/2} \times\exp\left[-\frac{ie}{\hbar c}\mathbf{A}\cdot\boldsymbol{\rho}\right]\mathcal{J}_\sigma(\rho,\omega_\nu) , \tag{19}$$

where

$$\mathcal{J}_\sigma(\rho,\omega_\nu)=2i\pi\operatorname{sgn}(\omega_\nu)\exp\left[i\frac{\rho}{a_H}\left[[(2n_0)^{1/2}+\mu_\sigma^F/(2n_0)^{1/2}]\operatorname{sgn}(\omega_\nu)-\frac{|\omega_\nu|}{\omega_c(2n_0)^{1/2}}\right]\right]\mathcal{J}_\sigma(\omega_\nu) \tag{20}$$

and

$$\mathcal{J}_\sigma(\omega_\nu)=1/\{1-\exp[-2\pi|\omega_\nu|/\omega_c+2\pi i\mu_\sigma^F\operatorname{sgn}(\omega_\nu)]\} . \tag{21}$$

Note that the integral over n' reduces to the pole contribution at $n'=\mu_\sigma^F+i\omega_\nu/\omega_c$, which represents a thermally broadened energy shell around the Fermi level. Thus the single-electron states which participate in pairing originate in many Landau levels around the Fermi energy rather than in a single, discrete level. Only at zero temperature may the semiclassical process of pairing be regarded as taking place on a single Landau level. This observation is consistent with the remark following Eq. (11) emphasizing the importance of the off-diagonal terms in the pairing process.

We are now ready to calculate the kernel Q [Eq. (5)]: Using Eqs. (5) and (19)–(21) and the identity

$$|\omega_\nu|/a_H\omega_c(2n_0)^{1/2}=|2\nu+1|/\zeta , \tag{22}$$

where $\zeta\equiv\hbar v_F/\pi k_BT$ is the thermal mean free path of an electron in the normal state, we find that

$$Q(\mathbf{r}_1,\mathbf{r}_2)=\left[\frac{2\pi k_BT}{k_F\rho}\right]\eta^2\exp\left[-\frac{2ie}{\hbar c}\mathbf{A}\left[\frac{\mathbf{r}_1+\mathbf{r}_2}{2}\right]\cdot\boldsymbol{\rho}\right] \times\sum_{\nu=0}^{\nu_D-1}\operatorname{Re}(q_\nu)e^{-\alpha_\nu\rho/a_H} , \tag{23}$$

where $\alpha_\nu\equiv 2(2\nu+1)a_H/\zeta$, and $\eta\equiv m_c/2\pi\hbar^2$ is the density of states in the 2D electron gas. In the above expression q_ν is given by

$$q_\nu=\frac{\exp[2\pi|\omega_\nu|/\omega_c+i\pi\operatorname{sgn}(\omega_\nu)\tilde{m}_c]}{\cos(2\pi n_F)+\cosh[2\pi|\omega_\nu|/\omega_c+i\pi\operatorname{sgn}(\omega_\nu)\tilde{m}_c]} , \tag{24}$$

where $\tilde{m}_c\equiv m_c/m_0$. This factor is responsible for the quantum oscillations.

Note that the imaginary frequency formalism used here is equivalent to the real frequency one only at discrete values of the temperature, for which ν_D is an exact integer. We therefore restrict the temperature in our calculations to such values. Note also that although our

derivation of Eq. (23) is in the Landau gauge, the result is expressed in a gauge invariant form.

The validity of Eq. (23) can be tested by checking whether the eigenfunction (8) of the exact kernel Q is also an eigenfunction of the approximate one given by Eq. (23). We find that the answer to this question depends on the gauge selected. In the symmetric gauge the "wave function" defined in Eq. (8) is an exact eigenfunction of our semiclassical kernel. Indeed, substituting Eqs. (8) and (23) into the left-hand side of Eq. (7), we find that

$$\int d^2r_2 Q(\mathbf{r}_1,\mathbf{r}_2)\Delta^*(\mathbf{r}_2)=(2\pi a_H k_B T/k_F)\eta^2 e^{-(1/2)z_1 z_1^*}\sum_{\nu=0}^{\nu_D-1}\mathrm{Re}(q_\nu)\Delta_0\int_0^\infty d\tilde{\rho}\, e^{-\alpha_\nu\tilde{\rho}-(1/2)\tilde{\rho}^2}\int_0^{2\pi} e^{z_1\tilde{\rho}e^{-i\theta}} f^*(z_1-\tilde{\rho}e^{i\theta})d\theta\ , \tag{25}$$

where $\tilde{\rho}\equiv\rho/a_H$. We now use the Taylor expansion of the entire function $f(z)$ about z_1:

$$f(z_1-\tilde{\rho}e^{i\theta})=f(z_1)+\sum_{n=1}^{\infty}\frac{\rho^n}{n!}e^{in\theta}f^{(n)}(z_1) \tag{26}$$

under the integral over θ in Eq. (25): For any $n\geq 1$ the integral vanishes, while for $n=0$ it is given by

$$\int_0^{2\pi} d\theta\, e^{z_1\tilde{\rho}e^{-i\theta}} f^*(z_1-\tilde{\rho}e^{i\theta})=2\pi f^*(z_1)\ . \tag{27}$$

With the help of this result Eq. (25) reduces to

$$\int d^2r_2 Q(\mathbf{r}_1,\mathbf{r}_2)\Delta^*(\mathbf{r}_2)=A_{\mathrm{sc}}\Delta^*(\mathbf{r}_1)\ , \tag{28}$$

where

$$A_{\mathrm{sc}}=2\eta\frac{a_H}{\xi}\sum_{\nu=0}^{\nu_D-1}\mathrm{Re}(q_\nu)\gamma_\nu \tag{29}$$

and

$$\gamma_\nu=\int_0^\infty d\tilde{\rho}\, e^{-\alpha_\nu\tilde{\rho}-(1/2)\tilde{\rho}^2}\ . \tag{30}$$

Thus the eigenfunction [Eq. (8)] of the exact quantum-mechanical kernel Q is also an exact eigenfunction of the semiclassical kernel derived here. The resulting expression for the eigenvalue, A_{sc}, has a very simple structure (discussed later). This simplicity is due to the analyticity of the entire function $f(z_1-\tilde{\rho}e^{i\theta})$, which leads, after integrating over θ, to a complete elimination of the $\tilde{\rho}$ dependence in Eq. (27). This leaves the Gaussian factor $e^{-(1/2)\tilde{\rho}^2}$ as a natural cutoff for $\rho>a_H$ in the integral over $\tilde{\rho}$. This is a very important observation: It confirms our *a priori* assumption that in the semiclassical limit the single-electron Green's function, appearing in the pair correlation function [Eq. (5)], can be approximated by the form (19), obtained under the assumption that $\rho^2\ll 8n_0a_H^2$. In this framework the pair propagator $Q(\mathbf{r}_1,\mathbf{r}_2)$ is constructed from pairs of electrons, which propagate from $\mathbf{r}_1$ to $\mathbf{r}_2$ in cyclotron orbits n,n', centered at the respective stationary points [Eq. (15)]:

$$x_0=\tfrac{1}{2}(x_1+x_2)\pm\sqrt{2n}\,a_H\Delta y/\rho \tag{31}$$

and x_0', which is obtained from x_0 by replacing n with n'. The distance between the two stationary points,

$$|x_0'-x_0|=a_H|(2n')^{1/2}\pm(2n)^{1/2}|\frac{|\Delta y|}{\rho}\ , \tag{32}$$

represents the projected distance between the centers of the two orbits on the x axis. There are two such distances corresponding to the $\pm$ signs in Eq. (32). For electrons near the Fermi surface the semiclassical conditions yield quite different length scales for these distances: One distance is much smaller than the magnetic length, a_H. The other distance is approximately $2(2n_F)^{1/2}a_H|\Delta y|/\rho\sim 2(2n_F)^{1/2}a_H$, that is about twice the cyclotron radius, which is much larger than a_H. Only the latter configuration is consistent with the conventional picture of Cooper pairing (see Fig. 1 in Ref. 13), since in this configuration the distance $\rho\equiv|\mathbf{r}_1-\mathbf{r}_2|$ between the intersection points of the two orbits is much smaller than the cyclotron radius $(2n_F)^{1/2}a_F$ and the short sectors of the orbits connecting these points are nearly parallel, satisfying approximately the standard condition of Cooper pairing: $\mathbf{k}'=-\mathbf{k}$. In this semiclassical picture the significance of the magnetic length a_H as a coherence length for the paired electrons is clearly understood: Only for propagation distances ρ which are of the order of a_H or smaller do the paired electrons remain coherent. Indeed, the Ginzburg-Landau definition of $H_{c2}(T)$, that is,

$$H_{c2}(T)=\phi_0/2\pi\xi^2(T)\ , \tag{33}$$

where $\phi_0\equiv hc/2e$ is the flux quantum, and $\xi(T)$ is the temperature-dependent Ginzburg-Landau coherence length, is equivalent to the equation

$$\xi^2(T)=a_H^2/2 \tag{34}$$

which shows that in the zero-field ($T\rightarrow T_c$) limit our coherence length for an arbitrary magnetic field tends to the Ginzburg-Landau result.

Now the self-consistency equation determining $H_{c2}(T)$ at any temperature $0<T<T_c$ can be written in our semiclassical approach as

$$\tilde{\alpha}\equiv 2(a_H/\xi)\sum_{\nu=0}^{\nu_D-1}\mathrm{Re}(q_\nu)\gamma_\nu-1/\lambda=0\ , \tag{35}$$

where $\lambda=V\eta$. The well-known low-field limit, that is, the BCS equation for T_c, is readily recovered by taking

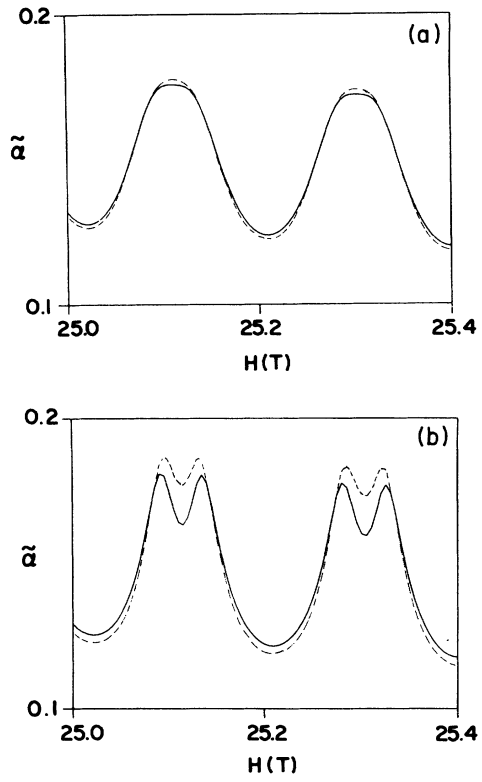

FIG. 1. A comparison between the semiclassical approximation used in this paper for the condensation energy $\tilde{\alpha}$ (solid curve) and the asymptotic expression derived by the Gruenberg-Gunther method (Ref. 11) (dashed-dotted curve), for two different temperatures: (a) $T=1$ K and (b) $T=0.5$ K. In these plots $\tilde{m}_c=2.22$, $E_F=2029$ K, and $T_c=87$ K.

the ratio a_H/ξ between the magnetic length and the thermal mean free path in Eq. (30) to be larger than unity. This amounts to taking $\alpha_\nu \gg 1$ and neglecting the quadratic term in the exponent with respect to the linear term. The integral over $\tilde{\rho}$ is then trivially performed to yield

$$\gamma_\nu \to 1/\alpha_\nu = \xi/2(2\nu+1)a_H \tag{36}$$

and, with the neglect of quantum oscillations (i.e., taking $q_\nu=2$), Eq. (35) reduces to

$$\sum_{\nu=0}^{\nu_D-1} \frac{1}{\nu+\frac{1}{2}} = \int_0^{\pi\nu_D} \frac{d\nu}{\nu} \tanh(\nu) = 1/\lambda \ , \tag{37}$$

the well-known BCS result.

It should be emphasized here that our semiclassical scheme is not identical to the conventional semiclassical scheme used by Gruenberg and Gunther:[11] In the latter the semiclassical condition $n_F \gg 1$ is invoked at the end of the derivation; that is, the exact quantum-mechanical result, Eq. (9), is calculated in the asymptotic limit. This can be done by using a Gaussian approximation for the combinatorial factor:

$$\frac{(n+n')!}{n!\,n'!\,2^{n+n'}} \approx (\pi n)^{-1/2} e^{-(n-n')^2/4n} \tag{38}$$

and by setting the lower limits of the summations over the Landau level quantum numbers, measured with respect to n_F, to be at $-\infty$. With the help of the Poisson summation formula and the residue method, one recovers our formula for A_{sc}, Eq. (29), with γ_ν identical to our result, Eq. (30), but with a slightly different formula for q_ν, that is,

$$q_\nu = 2 - 2\,\mathrm{Re}\left[\frac{1}{\epsilon e^{i\pi m_c/m_0}+1} + \frac{1}{\epsilon e^{-i\pi m_c/m_0}+1}\right] , \tag{39}$$

where

$$\epsilon = \exp(2\pi[\omega_\nu/\omega_c - i n_F]) \ . \tag{40}$$

We have compared the two results for q_ν and found that they are numerically very close, except for very low temperatures (see Fig. 1).

III. THE SUPERCONDUCTING STATE BELOW H_{c2}

A. The quartic term

To study the superconducting state below $H_{c2}(T)$ one should be able to calculate the quartic term in the free energy, Eq. (2), for a general variational form of the order parameter $\Delta(\mathbf{r})$. This is a complicated problem in the general case, but can be considerably simplified within our semiclassical approach due to our observation that paired electrons propagate coherently only within a distance much smaller than their cyclotron radii. Thus in calculating the quartic term we may take advantage of the fact that this term describes the propagation of four electrons where every one of them engages in pairing with two others [see Eq. (6)]. As a consequence this four-particle correlation process contributes significantly to the superconducting free energy only where the propagation distances of the four electrons involved are within a region of the order of the magnetic (coherence) length. It would therefore be sufficient to use our approximate form (19), for the single-electron Green's functions in the calculation of the quartic term.

Now, since those eigenfunctions of the integral operator Q [see Eq. (5)] which have the general form (8) constitute a complete set in the subspace of wave functions $\Delta(x,y)$, corresponding to the ground Landau orbital, Eq. (8) is the most general variational form of the order parameter when the condensate of Copper pairs is restricted to the ground Landau orbit. Substituting this variational form into Eq. (4), and using the approximate form, Eq. (19), of the single-electron Green's function, we can write the quartic term as

$$F_s^{(4)}=-B_0\Delta_0^4\int d^2r_1 d^2r_2 d^2r_3 d^2r_4(\tilde{\rho}_{12}\tilde{\rho}_{42}\tilde{\rho}_{13}\tilde{\rho}_{43})^{-1/2}f(z_1)f^*(z_2)f^*(z_3)f(z_4)$$
$$\times\exp\left[-\sum_{j=1}^{4}|z_j|^2/2\right]\exp\left[-\frac{i}{2}(\xi_{12}\Delta\eta_{12}+\xi_{42}\Delta\eta_{42}+\xi_{13}\Delta\eta_{13}+\xi_{43}\Delta\eta_{43})\right]$$
$$\times\exp\left[-\frac{i}{2}(\eta_{12}\Delta\xi_{12}+\eta_{42}\Delta\xi_{42}+\eta_{13}\Delta\xi_{13}+\eta_{43}\Delta\xi_{43})\right]$$
$$\times\sum_{\nu=-\infty}^{\infty}q_\nu^2\exp[i\,\mathrm{sgn}(\omega_\nu)(2n_F)^{1/2}(\tilde{\rho}_{42}-\tilde{\rho}_{12}+\tilde{\rho}_{13}-\tilde{\rho}_{43})-\tfrac{1}{2}|\alpha_\nu|(\tilde{\rho}_{42}+\tilde{\rho}_{12}+\tilde{\rho}_{13}+\tilde{\rho}_{43})]\,, \tag{41}$$

where $\tilde{\rho}_{ij}\equiv|\mathbf{r}_i-\mathbf{r}_j|/a_H$, $\xi_j\equiv x_j/a_H$, $\eta_j\equiv y_j/a_H$, $z_j\equiv\xi_j+i\eta_j$, $\xi_{ij}\equiv(\xi_i+\xi_j)/2$, $\Delta\xi_{ij}\equiv(\xi_i-\xi_j)$, and $B_0\equiv k_BT/32\pi^2\hbar^4a_H^{10}\omega_c^4n_F$. The use of the approximate form (19) will be further justified later on.

The entire function $f(z)$ can be written as[23]

$$f(z)=e^{(1/2)z^2}\sum_{n=-\infty}^{\infty}c_n\exp(2\pi inz/a_x)\,, \tag{42}$$

where $\{c_n\}$ are arbitrary variational coefficients, and a_x is an arbitrary, dimensionless constant. The sum over n defines an analytic function in the complex plane, which is periodic along the x axis. Since the period is of an arbitrary size a_xa_H, the proposed form of $f(z)$ can be used without loss of generality. The Gaussian factor $e^{(1/2)z^2}$ can be decomposed into an integral of the form

$$e^{(1/2)z^2}=\sqrt{2/\pi}\int_{-\infty}^{\infty}\exp(2mz-2m^2)dm \tag{43}$$

and so, $f(z)$ may be written as a Fourier-like expansion in the complex plane:

$$f(z)=\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty}c_n(m)e^{\omega_n^*(m)z}dm\equiv\sum\!\!\!\!\!\!\int_{\omega}c_\omega e^{\omega^*z}\,, \tag{44}$$

where $c_n(m)\equiv\sqrt{2/\pi}e^{-2m^2}c_n$ and $\omega_n(m)\equiv 2m-2n\pi i/a_x$.

The use of such a complex "Fourier" representation for the entire function $f(z)$ simplifies significantly the calculation of $F_s^{(4)}$. A further simplification may be achieved by noting that the above formula for $F_s^{(4)}$ contains factors of the form $\exp(i\tilde{k}_F^\nu\tilde{\rho}-\frac{1}{2}|\alpha_\nu|\tilde{\rho})/\sqrt{\tilde{\rho}}$, where $\tilde{k}_F^\nu\equiv\mathrm{sgn}(\omega_\nu)(2n_F)^{1/2}=k_Fa_H\mathrm{sgn}(\omega_\nu)$, which can be represented in the semiclassical limit as a Fourier integral:

$$\exp(i\tilde{k}_F^\nu\tilde{\rho}-\tfrac{1}{2}|\alpha_\nu|\tilde{\rho})/\sqrt{\tilde{\rho}}\to(2\pi)^{-3/2}e^{i\pi\,\mathrm{sgn}(\omega_\nu)/4}\int\frac{d^2\tilde{p}}{\sqrt{\tilde{p}}}\frac{e^{i\mathbf{p}\cdot\boldsymbol{\rho}}}{|\alpha_\nu|/2+i(\tilde{p}-\tilde{k}_F)\mathrm{sgn}(\omega_\nu)}\,, \tag{45}$$

where $\tilde{p}\equiv pa_H$.

Thus, representing each factor of this type by the Fourier integral (45), and using a combination of stationary phase and contour integration methods, we can reduce the multiple integral involved in the calculation of $F_s^{(4)}$ into a triple integral, and then write

$$F_s^{(4)}=-2\pi a_H^2\eta\left[\frac{a_H}{\zeta}\right]\left[\frac{a_H}{\xi_0}\right]^2\Delta_0^2\left[\frac{\Delta_0}{2\pi k_BT_c}\right]^2$$
$$\times\sum\!\!\!\!\!\!\int_{\omega_1,\ldots,\omega_4}c_{\omega_1}c_{\omega_2}^*c_{\omega_3}^*c_{\omega_4}e^{(1/2)\omega_{14}^*\omega_{23}}$$
$$\times\sum_{\nu=-\infty}^{\infty}q_\nu^2\int_0^\infty d\tilde{\rho}_{13}\int_0^\infty d\tilde{\rho}_{42}\exp[-|\alpha_\nu|(\tilde{\rho}_{42}+\tilde{\rho}_{13})-\tfrac{1}{4}(\tilde{\rho}_{42}+\tilde{\rho}_{13})^2]$$
$$\times\int_0^{\tilde{\rho}_{42}+\tilde{\rho}_{13}}d\tilde{\rho}_{12}\exp[-\tfrac{1}{4}(\tilde{\rho}_{12}-\tilde{\rho}_{42})^2-\tfrac{1}{4}(\tilde{\rho}_{12}-\tilde{\rho}_{13})^2]$$
$$\times I_0((\Delta\omega_{14}^*\Delta\omega_{23})^{1/2}\{[\tilde{\rho}_{12}-(\tilde{\rho}_{42}+\tilde{\rho}_{13})/2]^2+\tfrac{1}{4}(\tilde{\rho}_{42}-\tilde{\rho}_{13})^2\}^{1/2})\,, \tag{46}$$

where $\omega_{ij}\equiv(\omega_i+\omega_j)/2$, $\Delta\omega_{ij}\equiv(\omega_i-\omega_j)$, $\xi_0\equiv\hbar v_F/\pi k_BT_c$ is the zero-temperature coherence length, and I_0 is the modified Bessel function of zero order.

Note that in deriving this formula we have consistently neglected every term of $O((\Delta\omega_{ij})^2)$ or higher in the exponent. These terms are found to be either very small compared to unity (in the semiclassical limit), or of the order unity, but independent of the magnetic field. Since terms of this type are absent in the zero-field (classical Ginzburg-Landau) lim-

it, the field-independent ones should cancel each other, while the other ones are negligible.

Equation (46) shows that the contributions to the integrals over $\rho_{ij} \equiv |\mathbf{r}_i - \mathbf{r}_j|$ from regions where $\rho_{ij} \gg a_H$ are negligible. The dominant contributions to these integrals come from regions where $\rho_{ij} \leq a_H$, for which the approximation (19) for the single-electron Green's function is valid. Thus our use of the form (19) for the Green's functions in Eq. (6) is consistent with the result of the calculation presented in Eq. (46).

Using the integral representation

$$I_0(2\sqrt{ab}) = \int_0^{2\pi} \exp(ae^{i\theta} + be^{-i\theta}) d\theta$$

and performing the integrals over the real parts of ω_i, $i = 1,2,3,4$ we can rewrite Eq. (46) in the form

$$F_s^{(4)} = N\pi a_H^2 \eta \Delta_0^4 B \sum_{n_1,n_2,n_3} a_{n_1} a_{n_2}^* a_{n_3}^* a_{n_2+n_3-n_1} \times \sum_{\nu=0}^{\infty} \mathrm{Re}(q_\nu^2) \delta_\nu(n_2-n_1, n_3-n_1) \exp\left[-\left[\frac{\pi}{a_x}\right]^2 [(n_2-n_1)^2 + (n_3-n_1)^2] \right] , \tag{47}$$

where

$$a_{n_j} \equiv c_{n_j} e^{(\pi/a_x)^2 n_j^2} \tag{48}$$

are new variational coefficients, N is the total number of vortex lines threading the superconductor,

$$B \equiv 8 \left[\frac{a_H}{\zeta}\right] \left[\frac{a_H}{\xi_0}\right]^2 \Big/ \pi^{3/2} a_x (k_B T_c)^2 ,$$

and

$$\delta_\nu(n,n') \equiv \int_0^{\infty} d\tilde{\rho} \exp(-2\alpha_\nu \tilde{\rho} - \tilde{\rho}^2) \frac{1}{2\pi} \times \int_0^{2\pi} d\theta \int_{-\rho}^{\tilde{\rho}} dx \int_{-\tilde{\rho}}^{\tilde{\rho}} dy \exp\left[-(x^2+y^2)\sin^2\theta - ixy \sin(2\theta) + \frac{2\pi}{a_x}[y(in'\cos\theta - n\sin\theta) + x(-in\cos\theta + n'\sin\theta)] \right] . \tag{49}$$

B. Variational solutions

It is now possible, without any further approximation, to solve the variational equation derived from the free energy functional (2) with the quartic term given by Eq. (47). The quadratic term, Eq. (3), can be readily calculated with the help of Eqs. (28)–(30) to yield

$$F_s^{(2)} = -\pi a_H^2 N \Delta_0^2 \eta \tilde{\alpha} \sum_{n=-\infty}^{\infty} a_n^* a_n . \tag{50}$$

Thus, to fourth order in Δ_0, the superconducting free energy can be written in the following variational form:

$$F_s = \pi a_H^2 N \eta \Delta_0^2 \left[-\tilde{\alpha} \sum_n a_n^* a_n + \sum_{n_1,n_2,n_3} U(n_2-n_1, n_3-n_1) a_{n_1} \times a_{n_2+n_3-n_1} a_{n_2}^* a_{n_3}^* \right] , \tag{51}$$

where

$$U(n,n') \equiv \Delta_0^2 B \sum_{\nu=0}^{\infty} \mathrm{Re}(q_\nu^2) \exp[-(\pi/a_x)^2 (n^2+n'^2)] \times \delta_\nu(n,n') . \tag{52}$$

The free energy functional $F_s\{a_n, a_n^*\}$ in Eq. (51) describes an ensemble of particles (bosons), with condensation energy $\tilde{\alpha}$ per particle, but zero kinetic energy, interacting via a two-body potential $U(n,n')$ given by Eq. (52). The variational coefficients a_n, a_n^* may be regarded as annihilation and creation operators for those bosons. It should be noted here that Eq. (51) does not include any contribution to the free energy associated with the induced supercurrent. The leading contribution of this type is quadratic in Δ_0 but its prefactor is vanishingly small for the extremely type-II superconductors considered in this paper.

Variation of F_s with respect to the coefficients $\{a_n^*\}$ leads to the following equation for each n:

$$\tilde{\alpha} a_n = 2\Delta_0^2 B \sum_{n_1,n_2} \tilde{U}^r(n_2-n_1, n-n_1) a_{n_1} a_{n_2}^* a_{n+n_2-n_1} , \tag{53}$$

where

$$\tilde{U}'(n,n') \equiv \sum_{\nu=0}^{\infty} \mathrm{Re}(q_\nu^2)\exp[-(\pi/a_x)^2(n^2+n'^2)] \times \mathrm{Re}[\delta_\nu(n,n')] \ . \tag{54}$$

Equation (53) is a generalized version of the variational equation first derived by Abrikosov in his classic paper.[21] We have found that it has a *continuum* of *exact* solutions, which can be written explicitly in the form

$$a_n = \exp\left[\left[\frac{i\pi b_x}{a_x}\right]n^2\right] , \tag{55}$$

where b_x is an arbitrary real number, provided that the amplitude Δ_0 of the order parameter is the real positive solution of the quadratic equation:

$$\Delta_0^2 = \tilde{\alpha}/2Bs(b_x,b_y) , \tag{56}$$

$$s(b_x,b_y) \equiv \sum_{n,n'=-\infty}^{\infty} \tilde{U}'(n,n')e^{2\pi inn'b_x/a_x} = \sum_{n,n'=-\infty}^{\infty} \exp\left[-\frac{\pi b_y}{a_x}(n^2+n'^2)+\frac{2\pi i b_x}{a_x}nn'\right] \times \sum_{\nu=0}^{\infty} \mathrm{Re}(q_\nu^2)\,\mathrm{Re}[\delta_\nu(n,n')] \tag{57}$$

and $b_y \equiv \pi/a_x$. Note that at this stage b_x and a_x, and therefore also b_y, are completely arbitrary real numbers.

These solutions for the variational coefficients $\{a_n\}$ yield for the entire function $f(z)$:

$$f(z) = e^{z^2/2}\Theta_3\left[\frac{\pi z}{a_x}\middle|\frac{b}{a_x}\right] , \tag{58}$$

where $\Theta_3(\zeta|\kappa)$ is the Jacobi theta function,[24] and the complex number b is defined by $b \equiv b_x + ib_y$. The resulting solutions for the order parameter [see Eq. (8)] can be readily identified with the Eilenberger quasiperiodic eigenfunctions[25] for arbitrary 2D periodic lattices, whose primitive unit vectors are a_x and b. The relation between b and a_x, that is, $a_x b_y = \pi$, fixes the flux through each unit cell to be one flux unit ϕ_0. The remarkable thing about this set of solutions is that despite the inclusion of the quartic term in the free energy, the variational process does not favor any special geometry of the vortex lattice. Only the calculation of the free energy (51) for the various geometries of the vortex lattice can eventually isolate a single structure, like the triangular lattice: $b_x = \frac{1}{2}a_x$, $b_y = (\sqrt{3}/2)a_x$ as a favorable solution. Note that for any b_x of the form $b_x = (m+\frac{1}{2})a_x$, with m integer, our coefficients a_n [Eq. (55)] satisfy the Abrikosov periodicity conditions $a_{n+2} = a_n$, and $a_1 = ia_0$.[21]

To the best of our knowledge this is the first time one writes explicit expressions for the variational coefficients a_n (denoted c_n in Abrikosov's paper). It is remarkable that the same solutions are valid both in the (local) Ginzburg-Landau regime and in the (nonlocal) high-field regimes.

A useful approximate expression for $s(b_x,b_y)$ can be derived after noting that (1) For $n,n' \geq 1$ the contribution to the sums over n and n' in Eq. (57) is small, provided that b_y/a_x is not too small compared to unity; and (2) the dominant contribution to the integral over $\tilde{\rho}$ in Eq. (49) originates in $\tilde{\rho} < 1$. We may, therefore, regard the integration operator $(1/2\pi)\int_0^{2\pi} d\theta(\ )$ as an averaging $\langle\ \rangle$, and use a "cumulant" expansion of the average θ-dependent exponential in Eq. (49). Thus to second order in any combination of x,y,n,n' (note that $xy \leq \tilde{\rho}$) only the first cumulant of the θ-dependent exponent contributes and we find that

$$\delta_\nu(n,n') \approx 4\int_0^\infty d\tilde{\rho}\, e^{-2\alpha_\nu\tilde{\rho}-\tilde{\rho}^2} \times \int_0^{\tilde{\rho}} dx \int_0^{\tilde{\rho}} dy \exp[-(x^2+y^2)\langle\sin^2\theta\rangle] . \tag{59}$$

Now $\langle \sin^2\theta\rangle = \frac{1}{2}$ and the integrals over x and y can be readily performed analytically to yield

$$\delta_\nu(n,n') \approx 2\pi\int_0^\infty e^{-2\alpha_\nu\tilde{\rho}-\tilde{\rho}^2}[\mathrm{erf}(\tilde{\rho}/\sqrt{2})]^2 d\tilde{\rho} \equiv \delta_\nu . \tag{60}$$

Note that δ_ν is independent of n and n'. This reflects the fact that in the semiclassical approximation used the vortices and the superconducting electrons are separable entities. Consequently the double sum over n and n' in Eq. (57) can be readily carried out, leading to

$$s(b_x,b_y) = \tilde{s}(2b/a_x)\sum_{\nu=0}^{\infty}\mathrm{Re}(q_\nu^2)\delta_\nu , \tag{61}$$

with $\tilde{s}(\kappa) \equiv |\Theta_3(0|\kappa)|^2 + |\Theta_2(0|\kappa)|^2$ and $\Theta_{2,3}(\zeta|\kappa)$ the Jacobi theta functions.[24]

It can be readily shown that $(b_y/a_x)^{1/2}\tilde{s}(2b/a_x)$ is just the well-known geometrical factor β_A of the Abrikosov theory.[21,26] Thus our final result for the square amplitude of the order parameter can be written in the form

$$\Delta_0^2 = \frac{\tilde{\alpha}}{2\tilde{B}}(\pi k_B T_c)^2 , \tag{62}$$

where

$$\tilde{B} \equiv \beta_A\left[\frac{a_H}{\zeta}\right]\left[\frac{a_H}{\zeta_0}\right]^2\sum_{\nu=0}^{\infty}\mathrm{Re}(q_\nu^2)\delta_\nu . \tag{63}$$

Note that

$$\Delta_0^2 = (1/\pi N a_H^2)\int d^2r|\Delta(\mathbf{r})|^2 .$$

Thus Eq. (62) provides an explicit expression for the square modulus of the order parameter averaged over the entire Abrikosov vortex lattice.

The corresponding superconducting free energy per unit flux area can thus be written in the following Landau-like form:

$$f_s \equiv \frac{F_s}{N\pi a_H^2} = \eta\left[-\tilde{\alpha}\Delta_0^2 + \frac{\tilde{B}}{(\pi k_B T_c)^2}\Delta_0^4\right] = -\eta(\pi k_B T_c)^2\frac{\tilde{\alpha}^2}{4\tilde{B}} . \tag{64}$$

Note that $\tilde{B}$ [Eq. (63)] is proportional to β_A while the other factors in (63) are independent of the vortex lattice. Thus the free energy f_s for $\tilde{\alpha}>0$ is negative and inversely proportional to β_A, as in the classical Abrikosov theory.[18,26] This implies immediately that the triangular vortex lattice yields the minimum free energy.

An important test of our results for Δ_0^2 is to examine its zero-field (classical) limit: In this limit $(a_H/\zeta)\gg 1$, $q_\nu \to 2$, so that

$$\tilde{\alpha} \to \left[\int_0^{\pi\nu_D} \frac{d\nu}{\nu} \tanh(\nu) - 1/\lambda \right] ,$$

the well-known BCS result for $\tilde{\alpha}$. Furthermore, since $\alpha_\nu \gg 1$, and $T \to T_c$ in this limit:

$$\delta_\nu \to 2\pi \int_0^\infty e^{-2\alpha_\nu \tilde{\rho}} [\mathrm{erf}(\tilde{\rho}/\sqrt{2})]^2 d\tilde{\rho}$$
$$\to 4 \int_0^\infty e^{-2\alpha_\nu \tilde{\rho}} \tilde{\rho}^2 d\tilde{\rho} = \frac{1}{\alpha_\nu^3} \tag{65}$$

and

$$\tilde{B} \to \tfrac{1}{2}\beta_A \sum_{\nu=0}^{\infty} (2\nu+1)^{-3} = \tfrac{1}{2}\beta_A \frac{7\zeta(3)}{8} , \tag{66}$$

where $\zeta(n)$ is the Riemann zeta function. Thus the order parameter

$$\Delta_0^2 \to \frac{\tilde{\alpha}}{\beta_A [7\zeta(3)/8]} (\pi k_B T_c)^2 , \tag{67}$$

which is the well-known Gorkov results near T_c.

IV. BEYOND WKB

The WKB approximation used in this paper yields a remarkable agreement with the exact quantum-mechanical calculation of the condensation energy even quite close to the quantum limit (see Fig. 2). This should not be surprising since it is well known that for harmonic oscillators the semiclassical path integral is identical to the exact quantum-mechanical one.[27]

There are, however, some small, though systematic deviations, which reflect the sensitivity of the condensation energy to the presence of the cutoff in the pairing energy spectrum. As already indicated in Sec. II, the cutoff may be introduced in two alternative ways, which are not equivalent. Physically the procedure which leads to Eq. (11) should be the correct one since the cutoff is introduced to the real pairing energies there. Our WKB scheme is associated, however, with the alternate approach, where the cutoff is introduced to imaginary (Matsubara) energies.

We therefore consider here the difference ΔA between the corresponding quantum-mechanical expressions for the condensation energy:

$$\Delta A \equiv A - A_M , \tag{68}$$

where A is given by Eq. (11), and A_M is given by Eq. (9), with the Matsubara sum truncated at $|\nu| = \nu_D - 1$, that is,

$$A_M \equiv \tfrac{1}{2}\hbar\omega_c \sum_{n,n'=0}^{\infty} \frac{(n+n')!}{n!\,n'!\,2^{n+n'}} \left[\frac{\chi_\sigma(n)+\chi_{-\sigma}(n')}{\omega_c(n+n'+1)-2\mu} \right] , \tag{69}$$

with

$$\chi_\sigma(n) \equiv \tfrac{1}{2} \sum_{\nu=-\nu_D+1}^{\nu_D-1} \frac{1}{i\pi(\nu+\frac{1}{2}) - \frac{1}{2}\beta\varepsilon_{n,\sigma}} . \tag{70}$$

For Landau levels satisfying $\frac{1}{2}\beta|\varepsilon_{n,\sigma}| < \pi\nu_D$ the truncated Matsubara sum $\chi_\sigma(n)$ in Eq. (70) and the corresponding hyperbolic tangent in Eq. (11) are related by a contour integral over a circle of radius $\pi\nu_D$ in the complex plane (see Fig. 3), that is,

$$\chi_\sigma(n) = \tfrac{1}{2}\tanh(\beta\varepsilon_{n,\sigma}/2) - \mathcal{T}_{n,\sigma} , \tag{71}$$

with

$$\mathcal{T}_{n,\sigma} \equiv \frac{1}{4i\pi} \oint_{|z|=\pi\nu_D} \frac{\tanh(z)\,dz}{z - \frac{1}{2}\beta\varepsilon_{n,\sigma}} . \tag{72}$$

For Landau levels outside the circle $\chi_\sigma(n) = -\mathcal{T}_{n,\sigma}$.

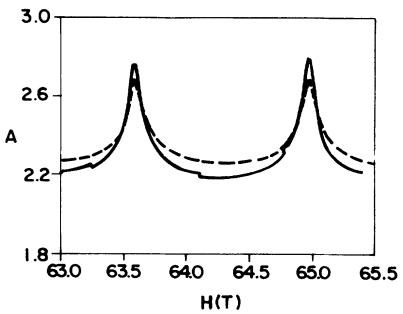

FIG. 2. A comparison between the semiclassical approximation used in this paper for the eigenvalue of the kernel Q (dashed curve) and the exact quantum-mechanical eigenvalue (solid curve). Note the small jumps in the exact result, which are due to the presence of the sharp cutoff. In this plot $T=0.75$ K, $\tilde{m}_c=2$, and the other parameters are as in Fig. 1.

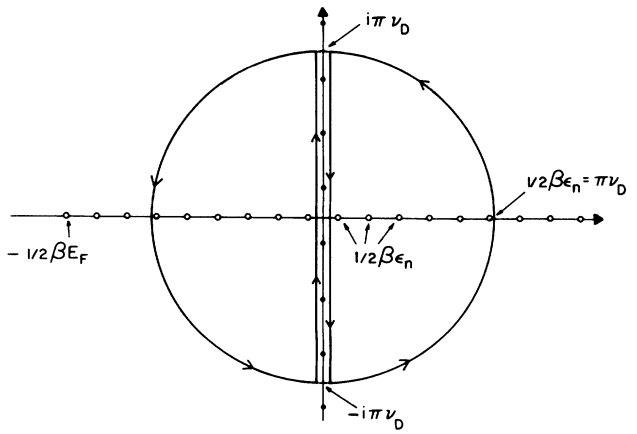

FIG. 3. The "cutoff" circle in the complex energy plane. The sense of integration along the contour is indicated by arrows. "Matsubara" frequencies are indicated along the imaginary axis, Landau levels along the real axis.

Thus the difference ΔA may be calculated from the expression

$$\Delta A = \tfrac{1}{2} \sum_{n,n'=0}^{\infty} \frac{(n+n')!}{n!\,n'!\,2^{n+n'}} \frac{\mathcal{T}_{n,\sigma}+\mathcal{T}_{n',-\sigma}}{n+n'+1-2n_F} \tag{73}$$

once the contour integrals $\mathcal{T}_{n,\sigma}$ are computed.

The behavior of ΔA when the field is varied can be studied by inspecting these integrals. Assuming, for simplicity, that the spin splitting is zero, the integrand has a simple pole whenever a Landau level crosses the cutoff circle (see Fig. 3). This happens when $\hbar\omega_c(n+\frac{1}{2}) = E_F \pm \pi k_B T_D$. Thus the sum over the Landau levels is dominated by the levels nearest to the circle edges (defined as the intersections between the circle and the real axis). It can be checked that the contributions from the levels inside the circle are positive while the levels outside the circle contribute negative amounts to ΔA (see Fig. 4). Now, by increasing the magnetic field, all the Landau levels move to the right on the real energy axis: Near the left edge of the circle, the internal level moves away from the edge, while the external one moves toward the edge, both leading to a monotonic decrease in ΔA. Near the right edge of the circle, however, the internal level moves toward the edge while the external level moves away from the edge, leading to a monotonic increase in ΔA. As soon as a level crosses a circle edge, there is a jump in the integral associated with the pole of the corresponding integrand. For the left edge, the corresponding jump in ΔA is positive since the level is entering the circle, while for the right edge the jump is negative since the level is leaving the circle. The remarkable aspect of this intriguing behavior (see Fig. 5) is that the rate at which levels cross the circle at the right edge is different from that at the left edge: The crossing rate at the right edge (i.e., above the Fermi energy) is $1+\pi k_B T_D/E_F$ times larger than the crossing rate at the Fermi energy (i.e., the dHvA frequency), while at the left edge (i.e., below the Fermi energy) the relative crossing rate is $1-\pi k_B T_D/E_F$.

All these lead to two beat frequencies in the dHvA oscillations of the condensation energy, associated with the presence of the cutoff in the pairing energy spectrum (see Fig. 5). The corresponding structures are temperature independent since the position of the levels with respect to the cutoff circle is independent of the temperature. They appear totally sharp since the cutoff in the simple BCS model used here is sharp.

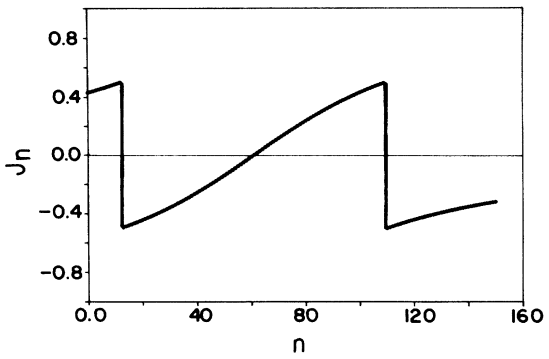

FIG. 4. The "cutoff" circle integral $\mathcal{T}_n$ [Eq. (72)] as a function of n, shown both inside and outside the pairing regions. Note the jumps at the circle edges.

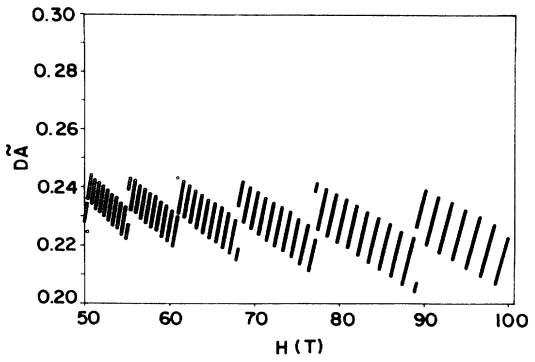

FIG. 5. Magnetic field dependence of the correction, ΔA, which should be introduced to the exact quantum-mechanical eigenvalue A_M after transferring the cutoff from the imaginary, thermal frequencies to the real energy spectrum. The values of the relevant parameters are $E_F = 2029$ K, $\pi T_D = 1640$ K.

One should keep in mind, however, that the nature of the cutoff depends on the pairing mechanism, and in any case cannot be totally sharp. For the conventional phononic mechanism it is far from being sharp. Thus the jumps should be smeared out in this case. Smooth oscillations, which reflect the entrance of Landau levels into the interaction region (the slow beating oscillations) may still be observable, however, at sufficiently high fields.

The frequencies of these oscillations are determined by the ratio $\pi k_B T_D/E_F$ of the cutoff energy to the Fermi energy: Larger cutoff energies make the fast oscillations (with respect to the dHvA oscillations) faster and the slow oscillations slower. A very large E_F makes the two beating frequencies closer to the central dHvA frequency (and to each other) and thereby leads to cancellations of the contributions from the incoming levels by those of the outgoing levels. Thus in the limit of a very large Fermi energy ΔA goes to zero. Note that in Eq. (73) ε_n varies between $-E_F$ and $+\infty$. This electron-hole asymmetry shifts the average value of ΔA from zero to some positive, nearly constant value when E_F is assumed to be a finite value. The zero-field limit ΔA_0 of ΔA is therefore not zero. Both our semiclassical expression A_{sc} [Eq. (29)] and the exact quantum-mechanical expression, Eq. (11), for A yield, however, the correct zero-field (classical) limit (37). Since A_{sc} is equivalent to the asymptotic limit of A_M [see the paragraph that follows Eq. (37)], it is surprising that the zero-field limit of the latter does not coincide with the BCS result (37).

This "paradox" can be resolved by noting that in deriving Eq. (19) for the single-electron Green's function the lower limit, $-n_0$, of the sum over the Landau levels [Eq. (16)] is replaced by $-\infty$. Clearly, for vanishing magnetic field $n_0 = [n_F]$ tends to ∞. However, the order in which one takes the limit turns out to be important: Keeping

the lower limit at $-n_0$ and then taking the zero-field limit yields a result which is smaller than the zero-field limit of (29) by the additive constant ΔA_0.

Thus our simple semiclassical expression for the condensation energy, Eq. (29), unlike the corresponding quantum-mechanical result (69), has the correct zero-field limit, and should be corrected only for the small quantum structures associated with the presence of the cutoff. This may be done by adding ΔA to A_{sc} and subtracting the average of ΔA over the period of the slow oscillations. Since this average is almost constant, very close to ΔA_0 (see Fig. 5), the corrected semiclassical condensation energy can be written as

$$A_{sc}^{cor} = A_{sc} + \Delta A - \Delta A_0 \ . \tag{74}$$

V. NUMERICAL RESULTS

The formalism developed in Secs. II–IV enables us to compute any observable which is a functional of the superconducting order parameter near the upper critical field. In particular, one may wish to compute the average magnetization per unit flux area, $M_s \equiv \partial f_s / \partial H$, due to the induced supercurrent, as a function of the magnetic field H. Since the Gorkov expansion is carried out around the normal-superconducting phase boundary, there is a significant zeroth-order contribution f_n to the total free energy $f = f_n + f_s$ associated with the normal electrons. The corresponding contribution, M_n, to the magnetization can be calculated analytically in the low-temperature (or high-field) limit, when only the two Landau levels adjacent to the Fermi energy are partially occupied.[28,29] The resulting expression for the magnetization[29] has an amplitude of the order of E_F/ϕ_0, so that the dimensionless quantity $\phi_0 M_n / E_F$ is of the order unity in this limit. The corresponding superconducting part of the magnetization may be written in this unit system as

$$\left[\frac{\phi_0}{E_F}\right] \frac{\partial f_s}{\partial H} = -H_{c2}(0) \frac{\partial(\tilde{\alpha}^2/2\tilde{B})}{\partial H} \ , \tag{75}$$

where $H_{c2}(0)$ is the zero-temperature upper critical field defined in Eq. (33). This result indicates that at fields H close to $H_{c2}(0)$ the superconducting and the normal parts of the magnetization are of the same order of magnitude. Our numerical results, shown in Fig. 6, confirm this conclusion. Since the magnetic field dependence of these two parts is quite different, it may be possible to distinguish between them. Thus measurement of the magnetization below $H_{c2}(T)$ at sufficiently low temperatures may be used as a tool for detecting quantum oscillations in the superconducting order parameter.

It should be noted here that under a strong magnetic field the chemical potential in systems, where the number of electrons is fixed, is not field independent.[28–31] In the 3D case the oscillatory part of the chemical potential has a prefactor of the order $1/n_F$ (Ref. 31) and is, therefore, small. In the 2D case, however, the oscillations may be quite strong, and should not be neglected. Their influence on the magnetization, as well as on other observables, such as the spin relaxation, has been investigated in detail in Refs. 28 and 32. In real 2D systems the strong oscillations of the chemical potential are, usually, damped due to various reasons, most of them are material dependent, and as such are very difficult to control. For example, the presence of a reservoir of electrons in localized states (e.g., in heterostructures), the existence of charge transfer between the intercalant and the conducting layers in some of the graphite intercalation compounds,[29] or the presence of several sheets in the Fermi surface, which is typical of most metals, strongly reduce the oscillations in the chemical potential. Furthermore, even when all these extrinsic factors are not present, the number of electrons cannot be assumed to be constant when Cooper-pair condensation takes place. A consistent calculation of the order parameter and the chemical potential is beyond the scope of this paper.

Thus, in the absence of a comprehensive scheme for calculating the chemical potential, it seems reasonable to examine the two extreme limits: (1) The limit when the number of electrons in Landau levels are fixed, and (2) the limit when the chemical potential is fixed. It is remark-

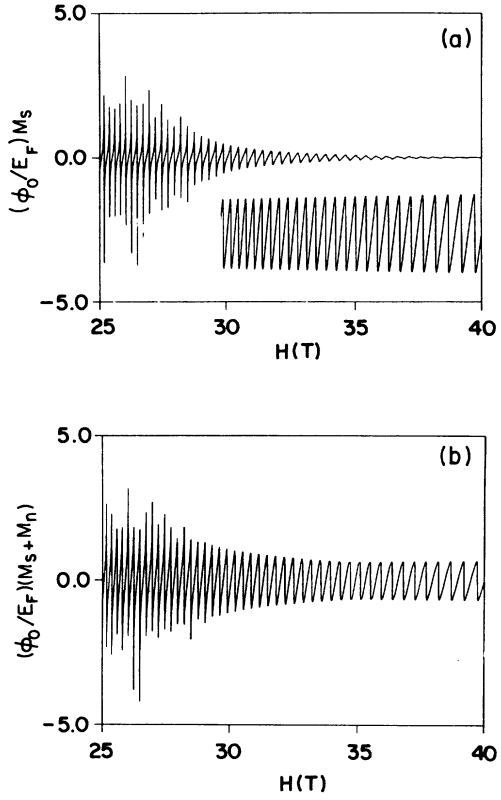

FIG. 6. (a) The superconducting magnetization oscillations in the limit of fixed number of electrons. The normal-electron part of the magnetization is shown in the lower right corner (shifted downward for clarity). The selected values of the parameters, i.e., $T_c = 87$ K, $E_F/k_B = 2029$ K, may characterize $Bi_2CaSr_2Cu_2O_{8+x}$. The mass ratio $m_c/m_0 = 2$ (second spin splitting zero), and $\pi T_D = 1093$ K. The temperature is $T = 1$ K. (b) The total (superconducting plus normal-electron) magnetization oscillations.

able that in both extremes we have found basically the same result; that is, in spite of the fact that many Landau levels are involved in the pairing, the superconducting order parameter is a strongly oscillating function of the magnetic field.

Figure 6 shows both the normal and the superconducting parts of the orbital magnetization below $H_{c2}(T=1\ \mathrm{K})$ in the case when the number of electrons is fixed. The selected values of the parameters used in the calculation may characterize the highly 2D Bi(2:1:2:2) oxide superconductor. As expected, it is seen that the envelope of the superconducting magnetization oscillations decreases with the magnetic field. What is remarkable, however, in this figure is the significant difference in the shape of the envelopes: While the normal magnetization envelope is seen to increase weakly with H in this field range, the superconducting magnetization envelope decreases exponentially with increasing magnetic field. This exponential behavior contrasts with the well-known linear decrease of the superconducting magnetization in the Ginzburg-Landau theory. There are also differences in the fine structures of the oscillations, which become very significant at lower temperatures (see Fig. 7).

A similar effect can be seen in the oscillations of the mean-square order parameter (Fig. 8). The value of the cyclotron effective mass selected in this figure (i.e., $m_c/m_0=2$) corresponds to zero spin splitting (see later). It is seen that by lowering the temperature the regions of large superconducting order expand, as expected, but also get flatter and eventually develop dips in the middle. The reason for this behavior can be understood by considering separately the corresponding oscillations of both $\tilde{\alpha}$ and $\tilde{B}$ [see Fig. 8(b)]. Since Δ_0^2 is proportional to the ratio $\tilde{\alpha}/\tilde{B}$, it is clear that any sharp change in $\tilde{\alpha}$ is compen-

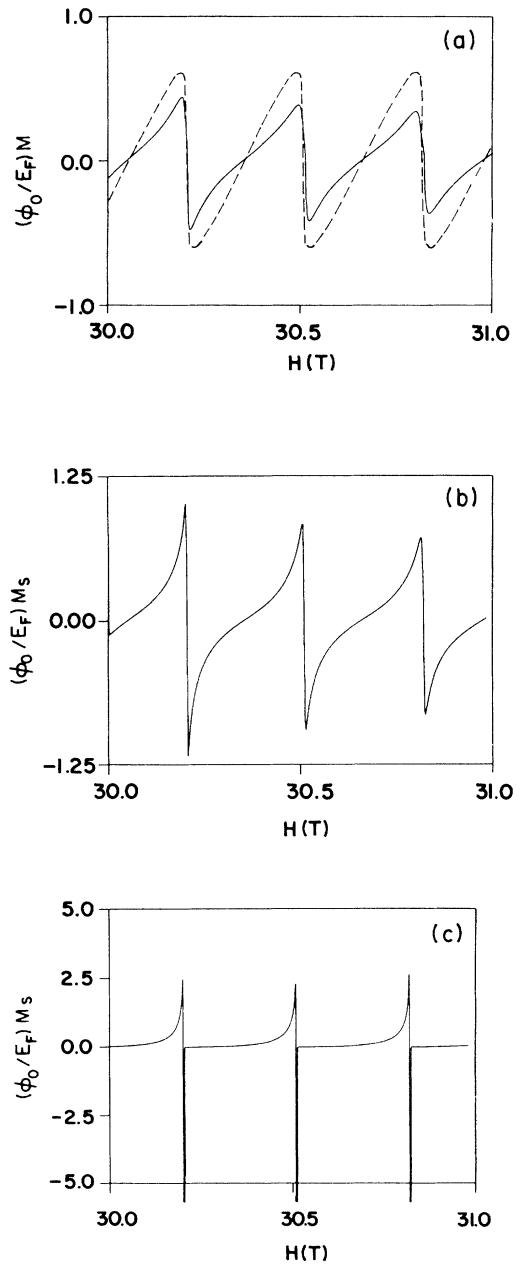

FIG. 7. (a) shows the same data as Fig. 6(a) within a small window of magnetic fields. The normal-electron part is represented by the dashed curve. (b) and (c) are plots similar to the superconducting part (solid curve) shown in (a) but with temperatures $T=0.75$ and 0.5 K, respectively. Note the flattening of the superconducting magnetization at low temperatures.

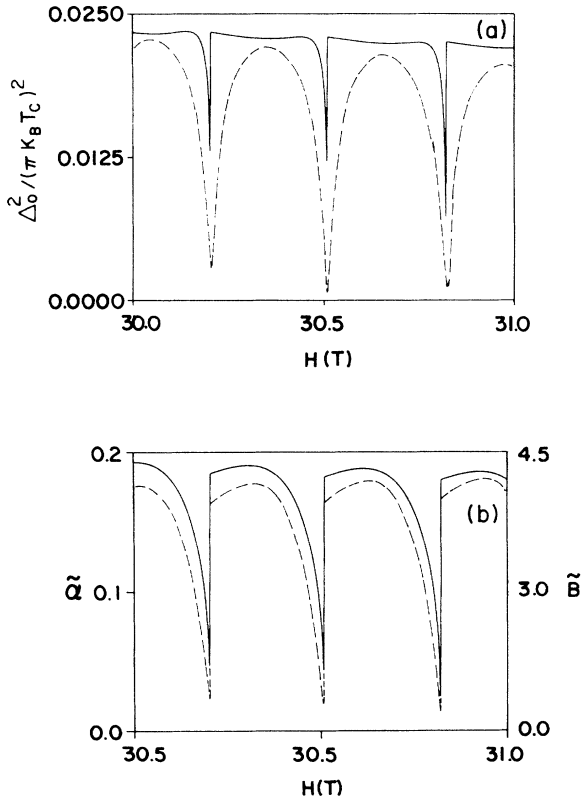

FIG. 8. (a) The mean-square order parameter within the same field range as in Fig. 7, and for the same set of parameters. The dashed curve is for $T=1$ K while the solid one is for $T=0.5$ K. (b) exhibits the condensation energy $\tilde{\alpha}$ (solid curve) and the pair-pair interaction factor $\tilde{B}$ (dashed curve), corresponding to the data presented in (a).

sated by the corresponding sharp change of $\tilde{B}$. This is a negative feedback effect on the sharp change of the density of states at the Fermi energy, which is associated with the interaction (quartic) term in the free energy (64). In other words, any sharp increase (decrease) in the density of states at the Fermi energy, which follows a variation in the magnetic field, leads to a sharp increase (decrease) in the condensation energy while also leading to a sharp increase (decrease) in the vortex-vortex repulsion. Thus the feedback is always negative and its strength increases with decreasing temperature since the interaction term varies with the square of the two-particle oscillation factor q_ν [see Eq. (63)], while the condensation energy term is only linear in this quantity.

Figure 9 exhibits data equivalent to Fig. 7 in the opposite extreme case when the chemical potential rather than the number of electrons is fixed. In contrast to Fig. 7, the regions of smooth variation correspond here to regions of low density of states [and low superconducting order; see Fig. 8]. Note that the oscillations exhibited in Fig. 9 are significantly smoother than the corresponding ones shown in Fig. 7. The sharp variation of the latter is restricted to certain narrow regimes, where the chemical potential changes rapidly between two adjacent Landau levels, and is the direct consequence of this motion.

Thus the dHvA oscillations arising solely from the Landau quantization of the pairing energy spectrum (and not from the oscillations of the chemical potential) are reflected in the magnetization curve of Fig. 9. They are, therefore, significantly smoother than the corresponding normal dHvA oscillations. This remarkable difference is due to the fact that the cooperative process of pairing involves many Landau levels around the Fermi energy, while in the normal state of our 2D system the presence of magnetic gaps in the single-electron spectrum makes the contributions of distant Landau levels exponentially small with $\hbar\omega_c/k_BT$. Quantitatively speaking, the thermal damping of the oscillating factors, q_ν [Eq. (24)], in the superconducting condensation energy, varies with $\exp[(2\pi^2 k_B T/\hbar\omega_c)|2\nu+1|]$. This is the usual Lifshitz-Kosevich factor,[33] which characterizes Landau-quantized systems without magnetic gaps (e.g., three-dimensional systems).

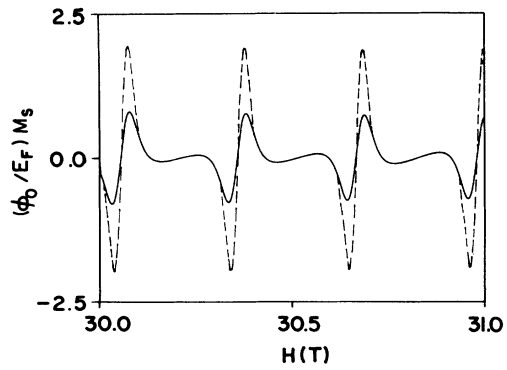

FIG. 9. (a) shows the superconducting magnetization oscillations, as in Fig. 7, but in the case when the chemical potential is fixed. The solid curve is for $T=1$ K, while the dashed curve is for $T=0.5$ K.

The oscillations in observables, which are functionals of the order parameter, are further smoothed out by the negative feedback effect discussed above. Nevertheless, at reasonably low temperatures the oscillations are quite strong, and persist well below H_{c2}, even in the usual situation, when the Zeeman spin splitting leads to pair breaking effect (see Fig. 2 in Ref. 13). Such large oscillations in Δ_0^2 around H_{c2} may lead to periodic disappearance and reentrance of superconductivity with $1/H$, which may result in a significant smearing of the transition to the superconducting state.

The oscillations enhance dramatically under the resonance (spin splitting zero) condition, when m_c/m_0 becomes close to an integer. The possibility of controlling experimentally the cyclotron mass to achieve such a resonant condition is unique to highly 2D electron systems; it can be done by tilting the magnetic field with respect to the axis normal to the conducting planes. Indeed, very recently Wosnitza *et al.*[34] reported measurements of the dHvA effect in organic superconductors, in which they determined up to four spin splitting zeros in the dHvA signal. Under such a resonant condition, the enhancement of the density of states at sufficiently high fields can be so large that the resulting increase in the superconducting condensation energy can compete with the in-

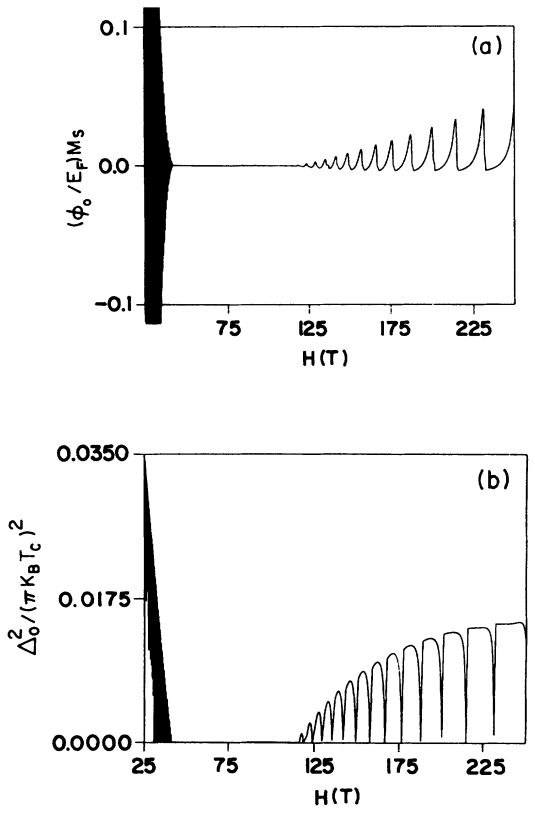

FIG. 10. (a) The superconducting magnetization and (b) the mean-square order parameter, for the same parameters as in Figs. 7(a) and 8(a) but in an extended field range up to 240 T. Note the considerably smaller amplitudes of the oscillations in the reentrance region.

crease of the pair kinetic energy, thus leading to a dramatic reentrance of the superconducting state well above the classical Ginzburg-Landau phase boundary.

In Fig. 10 we exhibit numerical results for the magnetization M_s and for the mean-square order parameter over an extended field range up to 240 T, and for $T=1$ K. The mass ratio in this plot is 2. The remarkable feature of this plot is the reentrance of the superconducting dHvA oscillations above 120 T, well above the classical phase boundary. Note, however, that the oscillation amplitudes in the reentrance region are much smaller than in the conventional superconducting region. The corresponding phase diagram is shown in Fig. 11(e). The critical point for the backbending of the phase boundary is found at about $T=0.8$ K and $H=50$ T, which is within an experimentally accessible range of fields and temperatures. This is a dramatic manifestation of the two-dimensional dHvA effect since the critical temperature for the backbending in three dimensions is several orders of magnitude lower.[3,5] For comparison, the phase diagrams for higher-order spin splitting zeros are also shown in Fig. 11: The critical temperature seems to be independent of mass ratio, whereas the critical field increases linearly with it. It should be noted, however, that a small deviation from zero spin splitting is sufficient to diminish this reentrance effect [see Fig. 11(d)].

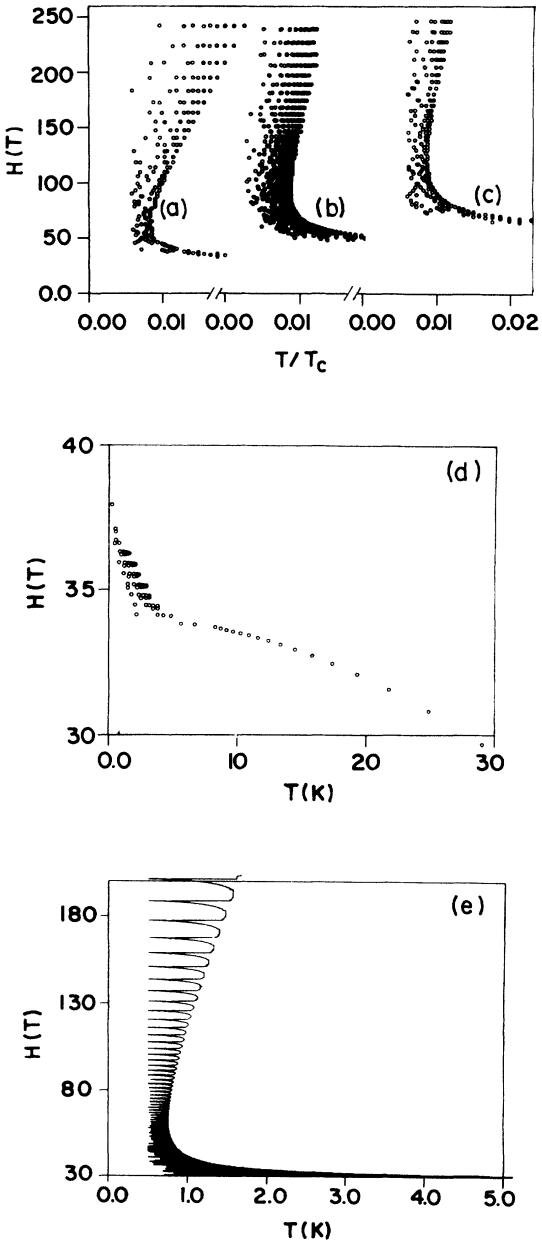

FIG. 11. Phase diagrams around the critical points for reentrance superconductivity for three spin splitting zeros: (a) $m_c/m_0=2$, (b) 3, and (c) 4. (d) A similar plot for nonvanishing spin splitting ($m_c/m_0=2.22$). The chemical potential is fixed in these plots. (e) The same as (a) but with the number of electrons fixed.

The extraordinary aspects of the 2D dHvA effect predicted in this paper are all expected to be washed out by sufficiently strong impurity scattering. This will take place by smearing the oscillation factors q_ν in the same way as in the ordinary dHvA effect. This smearing effect can thus be estimated in terms of a Dingle temperature. The thermal broadening of the oscillations, calculated in this paper, indicates that such a Dingle temperature should not exceed a value of about 1% of T_c to avoid smearing the main oscillations' effects.

Fluctuations pose another challenge to the observation of the predicted effects. The ordinary amplitude and phase fluctuations of the order parameter should be strongly quenched by the low temperatures (and high fields) to be employed. The effect of vortex-line fluctuations[35] is far more difficult to estimate. Physically speaking, however, the oscillations considered here originate in the underlying single-electron quantization structure near the Fermi surface, which is not expected to be strongly affected by spatial variations in the (small) order parameter near H_{c2}. Furthermore, the remarkable decoupling found in Sec. III, between the oscillatory part of $\tilde{B}$ and the part associated with the vortex lattice, may indicate that vortex-line motion should not strongly affect the oscillations in Δ_0^2.

VI. CONCLUSION

In this paper we have studied the extremely type-II superconducting state of a 2D electron gas under high magnetic fields near H_{c2}, focusing on the calculation of physically measurable quantities, such as magnetization oscillations. In addition to the physical predictions of this paper, we have gained a deeper insight into the behavior of 2D superconductors in magnetic fields. We have found that the conventional picture of pairing is not drastically changed under the influence of a strong magnetic field, provided that the number of occupied Landau levels is large: As long as this number is not too close to unity, the pairing coherence length is much shorter than the cyclotron radius of an electron at the Fermi energy, and the dominant pairing processes take place between electrons of approximately equal and opposite momenta. The single-electron states involved in pairing originate in many Landau levels around the Fermi energy, and they

effectively appear as a thermally broadened energy shell around the Fermi energy. Pairing at low but finite temperatures should therefore be regarded as both intra- and inter-Landau-level processes.

Contrary to the analysis of Ref. 15, we have found that the crossover between the semiclassical and the quantum regimes is quite smooth, and that "semiclassical pairing" remains an appropriate picture rather deep inside the quantum regimes. This result may have important implications in related areas. For example, very recently Dukan, Andreev, and Tešanović[17] considered the quasiparticle excitation energies in the quantum limit (i.e., when pairing is restricted to a single Landau level) and found that, due to the vanishing of the order parameter at the reciprocal lattice points of the vortex lattice, this energy spectrum is gapless. Since in the low-field limit the spectrum has a gap, it is clear that the inclusion of a sufficiently large number of Landau levels (i.e., off-diagonal terms) in the Bogoliubov–de Gennes equations should eventually reopen the gap in the quasiparticle energies. On the basis of our results it is therefore expected that the crossover from the conventional superconducting state to the very high-field gapless state would be quite smooth.

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