Self-consistent Bogoliubov–de Gennes theory of the vortex lattice state in a two-dimensional strongly type-II superconductor at high magnetic fields

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A self-consistent Bogoliubov–de Gennes theory of the vortex lattice state in a 2D strong type-II superconductor at high magnetic fields reveals a novel quantum mixed state around the semiclassical H_{c2} , characterized by a well-defined Landau-Bloch band structure in the quasiparticle spectrum and suppressed order-parameter amplitude, which sharply crossover into the well-known semiclassical (Helfand-Werthamer) results upon decreasing magnetic field. Application to the 2D superconducting state observed recently on the surface of the topological insulator Sb₂Te₃ accounts well for the experimental data, revealing a strong type-II superconductor, with unusually low carrier density and very small cyclotron mass, which can be realized only in the strong coupling superconductor limit.

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I. INTRODUCTION

The recent discoveries of surface and interface superconductivity with exceptionally high superconducting (SC) transition temperatures in several material structures [1-3]promise to stimulate fundamental studies of the phenomenon of strong type-II superconductivity in two-dimensional (2D) and quasi 2D electron systems, particularly under high magnetic fields [4]. In a pure strong type-II superconductor under a uniform magnetic field the quasiparticle spectrum is gapless in a broad field range below the upper critical field H_{c2} [4–6], where scattering of quasiparticles by the vortex lattice interferes with the Landau quantization of the electron motion perpendicular to the magnetic field to form magnetic (Landau) Bloch's bands. In pure 2D, or quasi 2D, strong type-II SC systems, such as that realized in the multilayer system of the organic charge transfer salt $\kappa - (ET)_2 Cu(SCN)_2$ [7], under a magnetic field perpendicular to the easy conducting plane, the underlying normal electron spectrum is fully quantized and the effect of the vortex lattice is very pronounced. 2D vortex lattices can realize in such strongly layered electronic systems due to the presence of weak crystalline disorder [8,9], where pinning of a few flux lines provide support for the entire vortex lattice against melting under an increasing magnetic field up to the irreversibility line [10]. Of special interest in the present paper is the unique situation of the 2D superconductivity realized in surface states of topological insulators, e.g., Sb₂Te₃ [11], where the chemical potential μ is close to a Dirac point [12] (with Fermi velocity v) and the cyclotron effective mass, $m^* = \mu/v^2$ [13], is a small fraction (e.g., 0.065 in Sb₂Te₃) of the free electron mass m_e , resulting in a dramatic enhancement of the cyclotron frequency, $\omega_c = eH/m^*c$, and the corresponding Landau level (LL) energy spacing.

Due to the suppressed energy dispersion along the magnetic field direction, characterizing the 2D electron system, and the particle-hole symmetry inherent to the SC state, the quasiparticle spectrum exhibits peculiar features that are missing in the 3D case. For example, at discrete magnetic field values where the chemical potential is located in the middle of a Landau band, so that the underlying normal state spectrum satisfies particle-hole symmetry, the calculated quasiparticle density of states shows a linear, Dirac-like energy dependence, which reflects topological singularities at the vortex lattice cores [4,14]. Both the enhanced Landau quantization effect and the lucid reflection of the topological singularity at the vortex-lattice cores in the quasiparticle spectrum [15,16] point to the great importance of self consistency in the theoretical description of 2D superconductors at high magnetic fields. The presence of well defined Landau bands in the quasiparticle spectrum, which is reflected as magnetoquantum (MQ) oscillations in the SC order parameter [17], via the self consistency equation, is expected to significantly alter the semiclassical picture of the SC phase transition at high magnetic fields [18]. In this paper we present results of systematic self-consistent solutions of the Bogoliubov-de Gennes (BdG) equations, which addresses these aspects of 2D superconductivity at high magnetic fields. It is, indeed, found that, due to self-consistency, the SC pair potential can be strongly distorted near the vortex-lattice cores and that the traditional semiclassical picture of a single critical point can be dramatically smeared into an intermediate state of quantum multicritical transition. The self-consistency formalism used here was first developed in Ref. [19]; however, its few past applications [19,20] have not addressed the novel aspects mentioned above.

II. THE MODEL

For the present analysis we consider a model of a 2D electron system under a perpendicular uniform magnetic field

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 $\mathbf{H} = (0,0,H)$, neglecting, for the sake of simplicity, any (Zeeman or spin-orbit induced) spin splitting and assuming a singlet, *s*-wave electron pairing. The large enhancement of the cyclotron energy in the physical model systems under consideration here [11] justifies this approximation (see below for more details).

The corresponding equations for the quasiparticle states in the mean-field approximation are the BdG equations in the Landau-orbitals representation, using the magnetic Bloch basis-set wave functions [5,19]:

$$\sum_{n'} \Delta_{n,n'}(\mathbf{q}) v_{n'}^N(\mathbf{q}) = (\varepsilon^N(\mathbf{q}) - \xi_n) u_n^N(\mathbf{q}), \tag{1}$$

$$\sum_{n'} \Delta_{n',n}^*(\mathbf{q}) u_{n'}^N(\mathbf{q}) = (\varepsilon^N(\mathbf{q}) + \xi_n) v_n^N(\mathbf{q}), \qquad (2)$$

where the single-electron (LL) energy measured relative to the chemical potential μ is given by $\xi_n = \hbar \omega_c (n - n_F), n =$ $0, 1, 2, ..., n_F = \mu/\hbar \omega_c - 1/2$. The matrix elements, $\Delta_{nn'}(\mathbf{q})$, of the self-consistent pair potential [4]:

$$\Delta(\mathbf{r}) = |V| \sum_{N} \sum_{\mathbf{q}} u_{\mathbf{q}}^{N}(\mathbf{r}) v_{\mathbf{q}}^{N*}(\mathbf{r}) \tanh(\varepsilon^{N}(\mathbf{q})/2k_{B}T) \quad (3)$$

are calculated by exploiting an expansion [5,21]:

$$\Delta(\mathbf{r}) = \sum_{j=0,1,2,\dots} \Delta_j \eta_j(\mathbf{r}) \tag{4}$$

in terms of Landau orbitals wave functions of a Cooper pair (charge 2*e*):

$$\eta_j(\mathbf{r}) = \sum_{k=0,\pm 1,\pm 2,\dots} e^{i\pi(\frac{b_x}{a_x})k^2} e^{i\frac{2\pi k}{a_x}x} \varphi_j \left[\sqrt{2}\left(y + \frac{\pi k}{a_x}\right)\right], \quad (5)$$

where $\varphi_j(y) \equiv (\sqrt{\frac{\pi}{2}}2^j j!)^{-1/2} e^{-\frac{1}{2}y^2} H_j(y)$, and $H_j(y)$ is Hermite polynomial of order *j*. Here $\mathbf{a} = (a_x, 0), \mathbf{b} = (b_x, b_y)$ are two primitive vectors in a general rhombic vortex lattice, forming a primitive unit cell of area $a_x b_y = \pi$, corresponding to one Cooper-pair flux quantum (note that all spatial lengths are measured in units of the magnetic length: $a_H \equiv \sqrt{\frac{ch}{eH}}$). Self-consistency is therefore established by requiring the coefficients Δ_j to satisfy the equations:

$$\Delta_{j} = \hbar \omega_{c} (\sqrt{2}\pi/a_{x}) (j!2^{j}) \lambda \sum_{n,m=n_{F}-n_{0}}^{n_{F}+n_{0}} \Gamma_{n,m}^{j} \times N_{\phi}^{-1}$$
$$\times \sum_{\mathbf{q}} \Phi_{nmj}(\mathbf{q}) \Psi_{n,m}(\mathbf{q})$$
(6)

where:

$$\Gamma_{n,m}^{j} \equiv 2^{-n-m} (n!m!)^{-1/2} (-1)^{m} \sum_{k=0}^{j} (-1)^{k} C_{k}^{m} C_{j-k}^{n}, \quad (7)$$

$$\Psi_{n,m}(\mathbf{q}) \equiv \sum_{N} u_n^N(\mathbf{q}) v_m^{N*}(\mathbf{q}) \tanh(\varepsilon^N(\mathbf{q})/2k_B T), \quad (8)$$

$$\Phi_{nmj}(\mathbf{q}) = \left(\sqrt{\frac{\pi}{2}} 2^{j} j!\right)^{-1/2} \\ \times \sum_{l=0,\pm 1,\pm 2,\dots} H_{n+m-j} \left[\sqrt{2} \left(q_{x} + \frac{\pi l}{a_{x}}\right)\right] \\ \times e^{i\pi (\frac{b_{x}}{a_{x}})l^{2} - i(\frac{2\pi l}{a_{x}})q_{y} - (q_{x} + \frac{\pi l}{a_{x}})^{2}}, \qquad (9)$$

 $n_0 \equiv [\omega_D/\omega_c], N_{\phi}$ is the number of flux lines threading the SC sample, and ω_D the (Debye) cutoff frequency, and the matrix elements: $\Delta_{nm}(\mathbf{q}) = \sum_{j=0}^{\infty} \Delta_{j,nm}(\mathbf{q})$, obeying the equations:

$$\Delta_{j,nm}(\mathbf{q}) = \Delta_{j}(2\pi)^{-1/4} (j!2^{j})^{1/2} \Gamma_{n,m}^{j} \\ \times \sum_{l} e^{-\frac{i\pi}{4} (\frac{b_{x}}{a_{x}})l^{2} + i\frac{2\pi l}{a_{x}} q_{y} - (q_{x} + \frac{\pi l}{a_{x}})^{2}} \\ \times H_{n+m-j} \bigg[\sqrt{2} \bigg(q_{x} + \frac{\pi l}{a_{x}} \bigg) \bigg].$$
(10)

Note the dimensionless coupling constant λ in Eq. (6), which is related to the effective electron-electron interaction parameter |V|, through: $\lambda \equiv |V|(m^*/2\pi\hbar^2) = |V|/2\pi a_H^2\hbar\omega_c$. Note also that the range of summation over the wave vectors **q** in Eq. (6) is restricted to the first magnetic Brillouin zone, which can be further reduced to a quarter, or one-sixth part of the zone, depending on whether the point symmetry of the vortex lattice is fourfold or sixfold, respectively.

III. SELF-CONSISTENT CALCULATIONS

A. Vortex core distortion

For the sake of simplicity, all numerical calculations have been performed here with the square-lattice geometry. The small changes associated with a different lattice geometry, e.g., the more common triangular geometry, are irrelevant to the purposes of the present paper.

The self-consistent solution code starts with initial values of the coefficients Δ_i in the expression for the matrix elements in Eq. (10), for which the calculated $4 \times (2n_0 + 1) \times (2n_0 + 1)$ BdG matrix in the $2 \times (2n_0 + 1)$ -dimensional vector space $(u_n^N(\mathbf{q}), v_m^N(\mathbf{q}))$ is numerically diagonalized at each point **q** in the magnetic Brillouin zone. The resulting eigenvectors and eigenvalues are then used to construct the pair potential for the next iteration with the new Δ_i and $\Delta_{nm}(\mathbf{q})$ through Eqs. (6) and (10), respectively. The iteration process continues until the values of Δ_j converge. Note that, due to the rotational symmetry of the vortex lattice, only Δ_j with j integer multiple of 4 (6) for the square (triangular) lattice are different from zero. The resulting values of Δ_i for j > 0, in the high magnetic fields region of well-defined Landau bands, are usually much smaller than $\Delta_{j=0}$, which corresponds to Abrikosov-lattice form of $\Delta(\mathbf{r})$, but become increasingly important upon decreasing the field below the crossover to a continuous spectrum, where the pair potential shows a reduced vortex core region and an oscillating behavior away from the core, which reflect the appearance of bound states [19]. Note, however, that at special small values of the LL filling factor $n_F + 1/2 (\propto 1/H)$, $\Delta_{j=2n_F}$ is strongly enhanced with respect to the other coefficients with j > 0, leading to a significant distortion of $\Delta(\mathbf{r})$ in the vortex core region, with



FIG. 1. (a) Self-consistent $|\overline{\Delta}_{SC}(\mathbf{r})|$ (i.e., measured in units of $\hbar\omega_c$), as a function of coordinate along the diagonal of the unit cell in the (square) vortex lattice (blue solid line), for $n_F = 9$. The other parameters used in the calculation are: $\lambda = 0.75$, $\hbar\omega_D/\mu = 0.2$, and $k_BT/\mu = 10^{-4}$. For comparison, the resulting $|\overline{\Delta}_{SC}(\mathbf{r})|$ calculated only with $\overline{\Delta}_{j=0}$, which corresponds to the Abrikosov solution, is also shown (dotted line). The inset shows all the nonzero $|\overline{\Delta}_j|$, j = $0,4,8,12,16 \leq 2n_F$. (b) Similar to (a) but for $n_F = 10$. The inset shows the nonzero coefficients $|\overline{\Delta}_j|$ at $j = 0,4,8,12,16,20 \leq 2n_F$. Note the parabolic distortion of $|\overline{\Delta}_{SC}(\mathbf{r})|$ in the vortex core region and the enhanced value of $|\overline{\Delta}_j|$ at $j = 2n_F$. For comparison, the resulting $|\overline{\Delta}_{SC}(\mathbf{r})|$, calculated without $\overline{\Delta}_{j=2n_F}$, is also included (red dashed line), showing no distortion of the vortex core region.

respect to the linearly vanishing Abrikosov form (see Fig. 1). The excess kinetic energy associated with this distortion is compensated by the extra condensation energy involved in the orbital extension over the reciprocal vortex lattice.

B. Magnetoquantum mixed superconducting state

Self-consistent determination of the pair-potential amplitude, Δ_{SC} , is also of a crucial importance in the range of relatively small n_F (high field) values, where MQ oscillations significantly influence the transition to the SC state. Figure 2



FIG. 2. Self-consistent order-parameter amplitude, $\overline{\Delta}_{SC}(n_F)$ (i.e., measured in units of $\hbar\omega_c$), calculated at integer values of n_F , for $\lambda = 0.75$ and different values of $\hbar\omega_D$ (0.2 μ —circles, 0.3 μ —diamonds, 0.4 μ —squares, and 0.5 μ —triangles). The corresponding best fitting curves to $\overline{\Delta}_{SC}(n_F)$, based on the GL-like expression are also shown (dashed lines).

shows $\overline{\Delta}_{SC}(n_F) \equiv \Delta_{SC}(n_F)/\hbar\omega_c$ [calculated at integer values of n_F , where $\Delta_{SC}(n_F)$ has maxima] for the coupling constant $\lambda = 0.75$ and various values of the cutoff frequency parameter $\hbar\omega_D/\mu$. The corresponding best fits of $\overline{\Delta}_{SC}(n_F)$ to a phenomenological Ginzburg-Landau (GL)-like formula:

$$\overline{\Delta}_{\rm GL}(n_F) \equiv \frac{\Delta_{\rm GL}(n_F)}{\hbar\omega_c} = (\gamma/n_{c2})n_F \left(1 - \frac{n_{c2}}{n_F}\right)^{1/2}$$
(11)

with two adjustable parameters, γ and n_{c2} , are also plotted in Fig. 2. The best fitting values of γ and n_{c2} are found to be close to $2\gamma_{\rm HW}$ and $2n_{c2}^{\rm HW}$, respectively, where:

$$\gamma_{\rm HW} \approx 0.56(\mu/\hbar\omega_D)\sinh(1/\lambda)$$
 (12)

and:

$$n_{c2}^{\rm HW} = \mu / \left(\hbar e H_{c2}^{\rm HW} / m^* c\right) = 0.563 (\mu / \hbar \omega_D)^2 \sinh^2(1/\lambda)$$
(13)

are the respective expressions derived within the semiclassical Helfand-Werthamer (HW) theory [18] for the order-parameter amplitude:

$$\overline{\Delta}_{\mathrm{HW}}(n_F) = \left(\gamma_{\mathrm{HW}}/n_{c2}^{\mathrm{HW}}\right)n_F \left[1 - \left(n_{c2}^{\mathrm{HW}}/n_F\right)\right]^{1/2}.$$
 (14)

Furthermore, the asymptotic $(n_F \rightarrow \infty)$ slope of $\overline{\Delta}_{GL}(n_F)$ in Eq. (11) for the best fitting parameters is found to be very close to the corresponding HW slope, that is:

$$\gamma/n_{c2} \simeq \gamma_{\rm HW}/n_{c2}^{\rm HW} = (\hbar\omega_D/\mu)/\sinh(1/\lambda)$$
 (15)

(see Fig. 3). Thus, both $\Delta_{GL}(n_F)$ and $\Delta_{HW}(n_F)$ tend in the zero field limit to the well known result for the SC energy gap, $\Delta = \hbar \omega_D / \sinh(1/\lambda)$. On the other hand, for n_F values below n_{c2} (i.e., for $H > H_{c2} = \mu m^* c / \hbar e n_{c2}$), where $\Delta_{GL}(n_F) = 0$, $\Delta_{SC}(n_F)$ deviates dramatically from the semiclassical theory, showing nonvanishing values, of magnitude comparable, or smaller than $\hbar \omega_c$. The novel quantum mixed SC state created in this field range is characterized by a cascade of normal to SC phase transitions, which crossovers to the usual SC state with



FIG. 3. Self-consistent order-parameter amplitude, $\overline{\Delta}_{SC}(n_F)$, (i.e., measured in units of $\hbar\omega_c$), calculated at integer values of n_F , for $\lambda = 1.0$, $\hbar\omega_D = 0.25 \,\mu$, and $k_B T = 2.5 \times 10^{-3} \,\mu$ (blue triangles), and the best fitting curve, based on the GL-like expression (blue dashed line). Also shown is the corresponding semiclassical (HW) result (magenta dashed line) and the self-consistent Landau bandwidth Δn_F (red diamonds). The scale for Δn_F on the right hand vertical axis. The horizontal red dotted segment indicates the saturation value (0.5) of Δn_F (for which the bands start to overlap).

a monotonically, steeply increasing order parameter amplitude for increasing n_F (decreasing H) values around n_{c2} (H_{c2}). This crossover closely follows the crossover of the quasiparticle spectrum from a well-defined Landau bands structure to a continuum, as can be seen in Fig. 3, where the width Δn_F of the Landau band at the chemical potential, defined by the interval of n_F values corresponding to nontrivial self-consistent solutions, is plotted as a function of integer n_F , together with $\Delta_{\rm SC}(n_F)$. It is remarkable that, in the entire fields range investigated, our calculations show that $\Delta n_F \simeq 0.2 \Delta_{\rm SC}(n_F)$, indicating that MQ oscillations, observed in the normal state, do not suffer appreciable additional damping upon entering the quantum mixed SC state. Significant effect of the SC order parameter on the MQ oscillations can be therefore observed only in the crossover region, as found experimentally in the organic superconductor $\kappa - (ET)_2 Cu(SCN)_2$ [4,22,23]. The filling factors range of this novel, quantum mixed SC state, estimated by:

$$n_{c2} - n_{c2}^{\rm HW} \approx n_{c2}^{\rm HW} = 0.563 (\mu/\hbar\omega_D)^2 \sinh^2(1/\lambda),$$

increases significantly (i.e., quadratically) with decreasing values of $\hbar \omega_D / \mu$ (see also Fig. 2), and much more sharply with decreasing values of λ .

IV. COMPARISON WITH EXPERIMENT AND CONCLUSION

Experimental evidence for the existence of the quantum mixed SC state discussed above can be found in results reported for the high field surface superconductivity observed recently in the topological insulator Sb₂Te₃ [11]. Using a simple s-wave BCS model of a 2D (circular) Fermi surface with the experimentally observed dHvA frequency, F = 36.5 T, and cyclotron mass $m^* = 0.065m_e$, and employing the basic dimensionless constants λ and $\hbar\omega_D/\mu$ of the model as adjustable parameters, we fit the zero field limit of the calculated self-consistent order parameter: $\Delta_{\rm SC}(n_F \to \infty) \to \hbar \omega_D / \sinh(1/\lambda)$ to the average SC energy gap derived from the STS measurements (i.e., $\simeq 13 \text{ meV}$) [11], and the semiclassical critical field $(n_{c2}^{\text{HW}} \approx 14, \text{ see Fig. 3})$ to the experimentally determined field of the resistivity onset downshift H_R (~2.5 T, $n_F \sim 14$) [11]. The resulting values of the adjustable parameters, $\lambda = 1$ and $\hbar \omega_D / \mu = 0.25$ imply strong coupling superconductivity with relatively small cutoff energy for the surface state of Sb₂Te₃.

Now, using the set of parameters selected above, we've calculated the self-consistent order parameter amplitude, $\Delta_{\rm SC}(n_F)$, at the temperature of the experiment, $T = 1.9 \text{ K}(k_BT/\mu = 2.5 \times 10^{-3})$, with the best fitting GL parameters; $\gamma = 5.8$, and $n_{c2} = 27$, showing an extended quantum mixed state region above the crossover field ($n_{c2} = 27$, see Fig. 3), characterized by small Landau bandwidth, $\Delta n_F \leq 0.1$, which seems to account for the puzzled, virtually normal state damping of the dHvA oscillation measured in this system below H_R [11].

It should be noted that the ideal model system considered here (by ignoring effects of disorder) is aimed at emphasizing the fundamental nature of our predictions, which could be clearly observed only in sufficiently pure materials. Nevertheless, the experimental results reported in Ref. [11] indicate that for the 2D superconductivity, realized in electronic surface states with Fermi energy near a Dirac point, the stringent purity conditions are dramatically relaxed due to the drastic suppression of the cyclotron mass. Thus, with $m^* = 0.065m_e$, the LL spacing of 5 meV at H = 3 T, exceeds the disorder scattering relaxation rate (~3 meV), observed in Sb₂Te₃. The large scale of the cyclotron energy can also justify, for the perpendicular field orientation employed in our model, the neglect of the Pauli paramagnetic limiting effect [24,25], originating in the rela-

tively large spin-orbit splitting, estimated to be about 1 meV in

Sb ₂Te₃. The latter remains smaller than $\Delta n_F \simeq 0.2 \Delta_{\rm SC}(n_F)$

shown in Fig. 3, even in the broad quantum multicritical region. In conclusion, we have shown here that in 2D electron systems with small cyclotron mass at the Fermi energy, where the effect of the magnetic field, through Landau quantization, is most pronounced, self consistency of the SC order parameter is crucial for understanding the transition to strong type-II superconductivity. In particular, the single critical-point picture of the SC phase transition, predicted by the mean-field semiclassical theory, is smeared into a finite range multicritical transition state, characterized by a well defined Landaubands structure in the quasiparticle spectrum and suppressed SC order parameter amplitude. Upon decreasing magnetic field below the semiclassical H_{c2} the quasiparticle spectrum crossovers sharply into a continuum and the order-parameter amplitude steeply approaches the well-known result predicted by the semiclassical (Helfand-Werthamer) theory. The fields range of this quantum mixed SC phase dramatically increases upon decreasing the pairing coupling constant λ , or cutoff energy $\hbar\omega_D$. It is therefore expected that observable MQ oscillations can be significantly affected by the SC order parameter only in the crossover region. This seems to be the reason for the rather sporadic appearance of this effect in the diverse literature reporting on dHvA oscillations in the SC state [4,26]. Our theory accounts reasonably well for the 2D SC state observed recently on the surface of the topological insulator Sb_2Te_3 [11], revealing a strong type-II superconductivity at unusually low carrier density and small cyclotron effective mass, which can be realized only in the strong coupling ($\lambda \sim 1$) superconductor limit. This unique situation is due to the proximity of the Fermi energy to a Dirac point, which implies that other materials in the emerging field of surface superconductivity, with metallic surface states and Dirac dispersion law around the Fermi energy, can show similar features.

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