

Phase transitions in vortex lattices of hexagonal exotic superconductors

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(Submitted 14 January 1992)

Zh. Eksp. Teor. Fiz. **101**, 1978–2000 (June 1992)

In this paper we suggest a theoretical description of magnetic phase transitions in hexagonal exotic superconductors with an order parameter having two complex components. For different values of magnetic field H and the Ginzburg–Landau functional coefficients we have qualitatively considered the problem of the energetically most favored structure of the vortex lattice near H_{c2} when \mathbf{H} is along the sixfold symmetry axis. Near H_{c2} a single-quantum lattice (SQL) could be regular triangular or rectangular. When the field decreases, a transition from a SQL to a two-quantum vortex lattice (TQL) is realized in the widest range of the functional coefficients. For further decrease in H a reverse TQL–SQL transition should occur in superconductors with a Ginzburg–Landau constant $\kappa \gg 1$. We have also found a coefficient range in which singular vortices are converted into nonsingular vortices. The values of the magnetic fields corresponding to these phase transitions are calculated as functions of the functional coefficients.

1. INTRODUCTION

The mixed state in superconductors with nontrivial pairing primarily associated with heavy-fermion superconductors can have some distinctive characteristics. For example, in Refs. 1–4 the anisotropy of the upper critical field in these superconductors was studied. The structure of vortices and vortex lattices for fields $H_{c1} < H < H_{c2}$ is also of great interest,^{3,5–12} since there is evidence of magnetic phase transitions in heavy-fermion superconductors. In UPt₃ such a transition has been discovered^{13–15} for $H \sim 0.6H_{c2}$. These experiments have been explained theoretically in Refs. 3, 5–12. The phase transitions in the mixed state can be related either to changes in the structure of separate vortices or to vortex lattice distortions. One of these theories involves a phase transition for fields H close to H_{c1} from a lattice of nonsingular single-quantum vortices, in whose core at least one of the components of the superconducting order parameter is non-zero to a lattice of singular vortices for H close to H_{c2} .^{7,9} In Ref. 7 the phenomenological Ginzburg–Landau (GL) equations have been solved numerically for a magnetic field along the anisotropy axis and it has been shown that nonaxisymmetric nonsingular vortices may exist near H_{c1} in a wide range of the functional coefficients. Then in Ref. 9 an analytic approach has been proposed to analyze the core structure of nonaxisymmetric singular and nonsingular vortices in exotic superconductors with symmetry groups D_{6h} and D_{4h} . This approach has allowed arbitrary orientations of \mathbf{H} relative to the crystal axes to be treated and the angular dependence of H_{c1} to be obtained. Another possible explanation of magnetic phase transitions has been proposed in Ref. 8. Using the Wigner–Seitz method of lattice energy calculation, it has been shown there that in a certain range of the GL functional coefficients a regular triangular lattice of two-quantum vortices is more favored than a regular triangular lattice of single-quantum vortices. Since near H_{c1} the latter are preferred from the energy standpoint in superconductors with a GL constant $\kappa \gg 1$, in Ref. 8 a transition from a single-quantum lattice (SQL) of vortices for low fields to a two-quantum lattice (TQL) for fields near H_{c2} has been suggested, but numerical calculations have shown that a transition

from a TQL in the intermediate H range to a SQL in fields of order H_{c2} is also possible.¹⁰

These magnetic transitions have been treated in Ref. 11 by a group theory approach and the formation of two- and three-quantum vortex lattices has been proposed.

In the present paper we quantitatively consider the preference, from the energy standpoint, of different vortex lattices near H_{c2} for a field H directed along the sixfold symmetry axis z and for a wide range of the coefficients of the GL functional corresponding to two-dimensional representations of the symmetry group D_6 . As is well known, trial functions, which are the solutions of the linearized GL equations for $H = H_{c2}$, are usually used in lattice energy calculations, and the superconducting seeds corresponding to the eigenfunctions of these equations for fields $H_n < H_{c2}$ are not taken into account near H_{c2} [$(1 - H/H_{c2}) \ll 1$]. This is undoubtedly true for superconductors with a single-component order parameter for which the intervals between the fields H_n are large [$H_n = H_{c2}/(2n + 1)$]. The lattice energy f^{GL} calculated in this approximation is of the order of $-(1 - H/H_{c2})^2$, the corrections being proportional to higher powers of the small parameter $(1 - H/H_{c2})$ (Ref. 16). In the case of a two-component order parameter one of the fields H_n (we will denote it by \tilde{H}) may be close to H_{c2} [that is, $(1 - \tilde{H}/H_{c2}) \ll 1$]. Then we must allow for superconducting seeds corresponding both to H_{c2} and \tilde{H} . As is shown below, the preferred vortex lattice can change with decreasing H field, which means that magnetic phase transitions exist.

In Sec. 2 we give and discuss the initial relations used below. In Sec. 3 we find the structure of the vortex lattice near H_{c2} for different values of the functional coefficients. The magnetic phase transitions, which occur when the field decreases, are considered in Sec. 4. The SQL–TQL transition, and the transition from a singular to a nonsingular lattice of single-quantum vortices, are found as functions of the field and functional coefficients. For superconductors with the GL constant $\kappa \gg 1$ a reverse TQL–SQL transition should occur, when H further decreases. The phase diagrams plotted in Sec. 4 allow us to reconcile the results of Refs. 8 and 10.

2. INITIAL RELATIONS

In the case when the superconducting classes for hexagonal crystals are generated by two-dimensional representations of the group D_6 , the order parameter has two complex components η_1 and η_2 . We write the GL functional in a magnetic field as follows:

$$f^{\text{GL}} = \int (-a\eta_1\eta_2 + b_1(\eta_1\eta_2)^2 + b_2|\eta_1\eta_2|^2 + K_1P_x\eta_1P_y\eta_2 + K_2P_x\eta_1P_z\eta_2 + K_3P_x\eta_1P_z\eta_2) dV, \quad (1)$$

$$P_x = P_y, \quad P_z = P_y, \quad \mathbf{P} = -i\hbar\nabla - 2e\mathbf{A}/c, \quad a = \alpha(T - T_c), \\ b_1 > 0, \quad b_2 > -b_1, \quad K_1 + K_2 + K_3 > |K_2|, \quad K_1 > |K_3|, \\ K_i > 0. \quad (2)$$

For $b_2 > 0$, a phase with broken time-reversal invariance occurs in the absence of a magnetic field. This corresponds to solutions with $(\eta_1, \eta_2) \sim (1, \pm i)$. For UPT₃ there are pieces of experimental evidence which indicate that precisely these phases exist.¹⁷ Therefore in what follows we limit ourselves to the case $b_2 > 0$.

For $\mathbf{H} \parallel z$ the solution of the linearized GL equations and the expression for H_{c2} have been found in Ref. 12. We change over from η_1, η_2 to Ψ_1, Ψ_2 according to the relations

$$\Psi_1 = (b_1/a)^{1/2}(\eta_1 - i\eta_2), \quad \Psi_2 = (b_1/a)^{1/2}(\eta_1 + i\eta_2). \quad (3)$$

The eigenfunctions have the form

$$(\Psi_{10}, \Psi_{20}) = (0, \varphi_0), \quad (\Psi_{11}, \Psi_{21}) = (0, \varphi_1)$$

and $\Psi_{1n} \sim \varphi_{n-2}$ and $\Psi_{2n} \sim \varphi_n$ for $n \geq 2$, where φ_n are the functions corresponding to the n th Landau level in the problem of electron motion in a magnetic field. The functions (Ψ_{1n}, Ψ_{2n}) are the solutions of the linearized GL equations only for definite values of the magnetic field $H = H_n$. Below we will need the expressions only for the two largest fields H_n :

$$H_0 = \frac{\hbar c}{2e\xi^2(1+C-D)}, \\ H_2^{\text{max}} = \frac{\hbar c}{2e\xi^2\{3(1+C) - 2[2C^2 + (1+C-D/2)^2]^{1/2}\}}, \quad (4)$$

where

$$\xi^2 = \hbar^2 K_1/a, \quad C = (K_2 + K_3)/(2K_1), \quad D = (K_2 - K_3)/(2K_1).$$

For $D > C^2/(1+C)$, we have $H_0 > H_2^{\text{max}}$ and, therefore, $H_{c2} = H_0$. The superconducting seeds arising for $H = H_{c2}$ are given by the functions Ψ_{10} and Ψ_{20} . If $D < C^2/(1+C)$, then $H_{c2} = H_2^{\text{max}}$ and the corresponding eigenfunctions are:

$$\Psi_{12} = \varphi_0, \quad \Psi_{22} = \gamma\varphi_2 = 0,5\gamma(P_x + iP_y)^2\varphi_0(L_H/\hbar)^2, \\ L_H = [\hbar c/(2eH)]^{1/2}, \quad \gamma = 0,5(1 - [1 + 2C^2/(1+C - D/2)^2]^{1/2})(1+C-D/2)/C. \quad (5)$$

It follows from (2) that $|\gamma| \leq 0.5$. We denote the smaller of two fields H_0 and H_2^{max} by \tilde{H} . As has been noted already in the Introduction, the fields H_{c2} and \tilde{H} may be close to each other (for sufficiently small values of C and D). Consequently, considering the vortex lattice near H_{c2} , it is necessary, in general, to allow for superposition of the functions (Ψ_{10}, Ψ_{20}) and (Ψ_{12}, Ψ_{22}) . However, for fields smaller than

H_{c2} but sufficiently large compared with \tilde{H} ($0 < 1 - H/H_{c2} \ll H/\tilde{H} - 1$) only the eigenfunctions corresponding to $H = H_{c2}$ need be taken into account. We will carry out these calculations in the next section.

3. VORTEX STRUCTURE FOR FIELDS CLOSE TO H_{c2}

In this section we study the vortex lattice structure in the field range $0 < 1 - H/H_{c2} \ll H/\tilde{H} - 1$. As mentioned above, the behavior of the order parameter (Ψ_1, Ψ_2) depends crucially on the values of the coefficients C and D . For $D > C^2/(1+C)$, the only nonzero component of the order parameter in this field range is Ψ_2 , and the lattice structure and energy are found in the same manner as in ordinary superconductors. Therefore we will consider here only the case $D < C^2/(1+C)$, when both Ψ_1 and Ψ_2 have nonzero values. For a vortex lattice with a unit cell in the form of a parallelogram enclosing a quantum of magnetic flux Φ_0 , the order parameter has the form

$$\Psi_1 = R \sum_n \exp(i\pi\rho n(n-1) + 2\pi inx/a_0 - 0,5((y - nb_0 \sin \alpha)/L_H)^2), \quad (6)$$

$$\Psi_2 = \gamma R \sum_n \exp(i\pi\rho n(n-1) + 2\pi inx/a_0 - 0,5((y - nb_0 \sin \alpha)/L_H)^2) \times (2((y - nb_0 \sin \alpha)/L_H)^2 - 1),$$

where $a_0 b_0 \sin \alpha = 2\pi L_H^2$, a_0 and b_0 are the parallelogram sides, α is the angle formed by these sides, $\rho = b_0 \cos \alpha/a_0$, and R is the constant given by the condition that the free energy be a minimum.

As pointed out in Ref. 8, in a certain coefficient range a two-quantum vortex lattice (TQL) can be energetically favored. Qualitatively, this possibility follows from the core structure of a single vortex near H_{c1} (Refs. 8,9). In this case the GL equations have an axisymmetric solution of the form

$$\Psi_1 = R_{1m}(r) \exp(im\theta), \quad \Psi_2 = R_{2n}(r) \exp(in\theta), \quad (7)$$

where m and n are related by the equation $m + 2 = n$, and (r, θ) are polar coordinates in the plane perpendicular to the vortex axis. If, for example, at large distances $\rho \rightarrow \infty$ the function R_{1m} is finite, a vortex contains m quanta of magnetic flux. It is important that in particular cases $m = -2$, $n = 0$ or $m = 0$, $n = 2$ either R_{1m} or R_{2n} is finite on the vortex axis, which means that two-quantum nonsingular vortices are possible. The core energy of such a nonsingular vortex could be smaller than the core energy of a singular single-quantum vortex. At the same time, for $\kappa \gg 1$ the energy related to superconducting currents in a vortex with m flux quanta is

$$f^{\text{GL}} \approx (m\Phi_0/(4\pi\lambda))^2 L \ln \kappa. \quad (8)$$

Here L is the vortex filament length, and λ is the magnetic field penetration length. The latter gives the main contribution to the single vortex energy, and, consequently, two-quantum vortices are energetically unfavorable for fields close to H_{c1} . We might, however, have a different situation for fields close to H_{c2} , when the distance between vortices is of the order of the core size. Therefore, considering the vor-

tex lattice structure, we must allow for the possibility of period doubling. We write the expression for the order parameter in the case, when the unit cell encloses two quanta of magnetic flux:

$$\Psi_1 = R \sum_n c_n \exp(2\pi i n x / a_0 - 0.5((y - n b_0 \sin \alpha) / L_H)^2),$$

$$\Psi_2 = \gamma R \sum_n c_n \exp(2\pi i n x / a_0 - 0.5((y - n b_0 \sin \alpha) / L_H)^2) \times (2((y - n b_0 \sin \alpha) / L_H)^2 - 1), \quad (9)$$

$$c_n = \theta_n \exp(i\pi \rho n(n-1)) = \begin{cases} \theta_{\text{even}} \exp(i\pi \rho n(n-1)), \\ \theta_{\text{odd}} \exp(i\pi \rho n(n-1)). \end{cases}$$

The upper expression is valid for even n , and the lower one for odd n . Note that for $\theta_{\text{even}} = \theta_{\text{odd}} = 1$ the formulae (9) reduce to (6). Arbitrary values of θ_{even} and θ_{odd} correspond to a lattice with two vortices of Ψ_1 per unit cell. In the case, when these vortices merge into one, we have a two-quantum vortex lattice.

Let us explain the terminology used. In the mixed state of a superconductor with a two-component order parameter there are vortices both of Ψ_1 and Ψ_2 . Given the function Ψ_1 , we can find Ψ_2 , so in what follows we will classify the solutions indicating only the type of the Ψ_1 vortex lattice. The expression (9) gives two types of Ψ_1 vortices: 1) single-quantum vortices for which the phase of Ψ_1 changes by 2π , when we go around the vortex axis, and 2) two-quantum vortices for which the phase changes by 4π . The lattice of vortices belonging to the first type will be called a single-quantum lattice (SQL), if the magnetic flux through its unit cell equals the quantum Φ_0 . The second type of vortices form a TQL lattice. The expression (9) describes also lattices of single-quantum Ψ_1 vortices with two flux quanta per unit cell, but in this case we will not introduce special notation.

Let us find the relation between the coordinates of the Ψ_1 vortices and the complex constants θ_{even} and θ_{odd} . The location of the zeros of the function Ψ_1 is schematically given in Fig. 1. Let (x_0, y_0) be the point where Ψ_1 vanishes. Equating expression (9) for Ψ_1 to zero, we find

$$\theta_{\text{even}} = - \sum_s \exp(i\pi \rho (2s-1)(2s-2) + 2\pi i (2s-1)x_0/a_0) \times \exp(-0.5((y_0 - (2s-1)b_0 \sin \alpha) / L_H)^2), \quad (10)$$

$$\theta_{\text{odd}} = \sum_s \exp(i\pi \rho 2s(2s-1) + 4\pi i s x_0/a_0 - 0.5((y_0 - 2s b_0 \sin \alpha) / L_H)^2).$$

For a SQL we have

$$x_{01} = a_0/2 + b_0 \cos \alpha, \quad y_{01} = -b_0 \sin \alpha/2. \quad (11)$$

Let us now find the coordinates of the zeros of the function Ψ_1 for a TQL. Note that the order parameter (9) does not change under inversion with respect to the points with coordinates

$$x' = (n+1/2)a_0 + b_0 \cos \alpha(1/2 - 2m), \quad y' = 2m b_0 \sin \alpha. \quad (12)$$

Therefore, the zeros of Ψ_1 are symmetric with respect to these points, where two Ψ_1 vortices merge into one (in the case of a TQL) for the following values of θ_{even} and θ_{odd} :

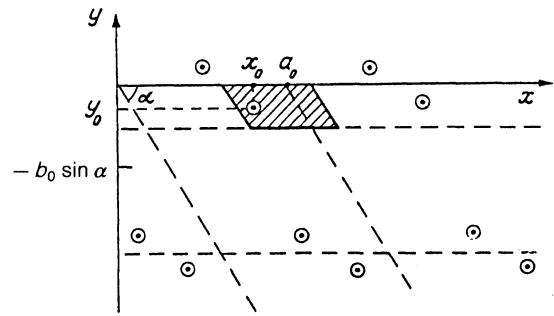


FIG. 1. Schematic location of the zeros of the function Ψ_1 in a lattice whose unit cell encloses two quanta of magnetic flux: $\rho = 0.3$, $\sigma = 0.5$, $x_0 = 0.8a_0$, $y_0 = -0.3b_0 \sin \alpha$, and \odot represents a zero of the function Ψ_1 .

$$\theta_{\text{even}} = \sum_s \exp(\pi(i\rho - \sigma)(2s-1)^2),$$

$$\theta_{\text{odd}} = \sum_s \exp(4\pi(i\rho - \sigma)s^2), \quad (13)$$

where $\sigma = b_0 \sin \alpha / a_0$.

Not only Ψ_1 does vanish at the points (x', y') , but also its derivatives with respect to x and y , which agrees with the asymptotic form (see Ref. 17)

$$|\Psi_1| \sim r^{-2}, \quad \text{where } r = ((x-x')^2 + (y-y')^2)^{1/2} \rightarrow 0.$$

Using the expressions (9) for Ψ_1 and Ψ_2 , we can find the lattice energy for $\kappa \gg 1$:

$$f^{\text{GL}} = j a^2 V / (2b_1) = - \frac{a^2}{2b_1} V (1 - H/H_{c2})^2 / (2\beta). \quad (14)$$

$$\beta = \frac{\langle |\Psi_1|^4 \rangle + \langle |\Psi_2|^4 \rangle + 2(1+2b) \langle |\Psi_1|^2 |\Psi_2|^2 \rangle}{\langle |\Psi_1|^2 + |\Psi_2|^2 \rangle^2}. \quad (15)$$

Here V is the superconductor volume, $b = b_2/b_1$, and the angle brackets in the expressions of a $\langle |\Psi|^2 \rangle$ type denote averaging over the volume. Further, it is necessary, generally speaking, to analyze the behavior of β as a function of ρ , σ , x_0 and y_0 . If we set γ to zero in (9), then Eqs. (14) and (15) will give the energy of a usual superconductor with a single-component order parameter. In this case, as is well-known, the free energy minimum (and, consequently, the minimum of the function β) corresponds to a regular triangular SQL ($\rho = 1/2$, $\sigma = 3^{1/2}/2$). Among all TQL with different ρ and σ the minimum of β also corresponds to a regular triangular TQL ($\rho = 1/4$, $\sigma = 3^{1/2}/4$).

For $\gamma \neq 0$ we will, therefore, compare the energies of regular triangular SQL and TQL. Such a comparison has been done in Ref. 8 by an approximate method similar to the Wigner-Seitz method and yields results in a simple analytic form. This method has been shown to give very good results for superconductors with a single-component order parameter.¹⁸ As a unit cell, we take a circle enclosing magnetic flux equal to the flux quantum Φ_0 for a SQL and $2\Phi_0$ for a TQL. Let us assume that the cell center coincides with the vortex lattice site, where the component Ψ_1 vanishes. To describe approximately the functions Ψ_1 and Ψ_2 inside the cell, we take the solutions of the linearized GL equations for $H = H_{c2}$ with a definite angular momentum. To this end, we

choose the gauge of the vector potential \mathbf{A} in the form $A_\theta = rH/2$, where (r, θ, z) is the cylindrical system of coordinates with the z -axis oriented along the magnetic field. For a SQL, the solution corresponding to H_{c2} has the form

$$\Psi_1 = (r/L_H) \exp(-i\theta - 0.25(r/L_H)^2), \quad (16)$$

$$\Psi_2 = 2\gamma(r/L_H)(1 - 0.25(r/L_H)^2) \exp(i\theta - 0.25(r/L_H)^2).$$

For a TQL we have

$$\Psi_1 = 0.5(r/L_H)^2 \exp(-2i\theta - 0.25(r/L_H)^2), \quad (17)$$

$$\Psi_2 = -2\gamma(1 - (r/L_H)^2 + 0.125(r/L_H)^4) \exp(-0.25(r/L_H)^2).$$

For a SQL the unit cell radius equals $r_1 = L_H\sqrt{2}$, and for a TQL it is $r_2 = 2L_H$. Using (16) and (17), we find β_1 and β_2 for the SQL and TQL respectively:

$$\beta_1 = (1.158 + 4.35\gamma^4 + 4.25(1+2b)\gamma^2)(1+2\gamma^2)^{-2}, \quad (18a)$$

$$\beta_2 = (1.332 + 8.62\gamma^4 + 3.153(1+2b)\gamma^2)(1+2\gamma^2)^{-2}. \quad (18b)$$

Setting β_1 equal to β_2 , we get a boundary in the $b\gamma$ plane separating the regions, in which regular triangular SQL or TQL are favored. The condition of TQL preference from the energy standpoint can be written in the form

$$D < C^2/(1+C), \quad b > (0.629p + 1.129 - 0.816(1+2p)^{1/2})/p, \quad (19)$$

$$p = C^2/(1+C-D/2)^2.$$

Due to conditions (2), $0 < p < 4$. For $b < b_n$, where $b_n \approx 0.28$ for any C and D satisfying Eqs. (2), a SQL is favored. Because of an arithmetic error, an incorrect value of the threshold b was obtained in Ref. 8. In reality, the region (19) where a TQL is energetically more favored than a regular triangular SQL is somewhat wider than that found in Ref. 8.

This method of β calculation assumes that the unit cell is well approximated by a circle of radius r_1 for a SQL and r_2 for a TQL. Such an approximation is valid only for regular triangular lattices. To determine the smallest β and the corresponding vortex configuration, it is necessary, however, to consider the case of arbitrary ρ , σ , x_0 and y_0 . Using (9), we find the following general expression for β :

$$\beta = 2\sigma^2(1+2\gamma^2)^{-2} (|\theta_{\text{even}}|^2 + |\theta_{\text{odd}}|^2)^{-2} \sum_{mn} (\theta_n^* \theta_n \theta_m \theta_{n+m}^* + \theta_{n+1}^* \theta_n \theta_{m+1} \theta_{n+m+1}^*) (1+2\gamma^2(1+2b)(0.75 - \pi\sigma(n^2+m^2) + \pi^2\sigma^2(m^2-n^2)^2) + \gamma^4(41/16 - 6.5\pi\sigma(n^2+m^2) + \pi^2\sigma^2(12.5(n^4+m^4) - 13n^2m^2) - 6\pi^3\sigma^3(n^2-m^2)^2(n^2+m^2) + \pi^4\sigma^4(n^2-m^2)^4)) \exp(-2\pi i nm \rho - \pi\sigma(n^2+m^2)). \quad (20)$$

For arbitrary fixed θ_{odd} , θ_{even} and σ the function β is periodic in ρ with a period 1 and satisfies the condition

$$\beta(\theta_{\text{odd}}, \theta_{\text{even}}, \sigma, 1-\rho) = \beta(\theta_{\text{odd}}, \theta_{\text{even}}, \sigma, \rho). \quad (21)$$

Therefore in finding the smallest β , it is sufficient to limit ourselves to the interval of a ρ change: $0 < \rho < 1/2$. Note also that for $\theta_{\text{odd}} = \theta_{\text{even}} = 1$ the lattice energy should not change, when the unit cell sides a_0 and b_0 are interchanged. Introducing a complex variable $\zeta = \rho + i\sigma$, we write this property in the form

$$\beta(\zeta) = \beta(1/\zeta^*). \quad (22)$$

Let us find now the range on which the coordinates

(x_0, y_0) of the component- Ψ_1 zeros vary in a lattice cell, which is necessary to consider studying β as a function of x_0, y_0 . Note the following properties of $\Psi_1(x, y, x_0, y_0)$:

$$\Psi_1(x, y, x_0, y_0) = \Psi_1(x, y, a_0 + b_0 \cos \alpha - x_0, -y_0),$$

$$\Psi_1(x, y, a_0/2 + b_0 \cos \alpha - x_0, -b_0 \sin \alpha/2 - y_0) \times \exp(-2\pi i(x_0/a_0 - x/a_0 + \rho)) = \Psi_1(x - b_0 \cos \alpha, y + b_0 \sin \alpha, a_0/2 + b_0 \cos \alpha + x_0, -b_0 \sin \alpha/2 + y_0), \quad (23)$$

$$\Psi_1(x - a_0/2, y, x_0 - a_0/2, y_0) = -\Psi_1(x, y, x_0, y_0).$$

Similar relations hold also for Ψ_2 . From these symmetry properties and Eq. (15), it follows that to find β as a function of x_0, y_0 , it is sufficient to consider the region shaded in Fig. 1 and given by the conditions

$$-b_0 \sin \alpha/2 < y_0 < 0, \quad (24)$$

$$a_0/2 + b_0 \cos \alpha/2 - y_0 \cot \alpha < x_0 < a_0 + b_0 \cos \alpha/2 - y_0 \cot \alpha.$$

We have found the minimum of the function $\beta(x_0, y_0, \rho, \sigma, b, \gamma)$ with respect to the variables x_0, y_0, ρ and σ by numerically summing the series (20). The results are shown in Fig. 2, where the regions are indicated in the $b\gamma$ plane, in which various types of SQL and TQL are energetically favored.

For the values of the parameters b and γ corresponding to the region 1, the minimum of β is realized for a regular triangular SQL ($x_0 = x_{01}, y_0 = y_{01}, \rho = 1/2, \sigma = 3^{1/2}/2$). At the boundary between the regions 1 and 2 the energy of this lattice becomes equal to the energy of a square SQL ($x_0 = x_{01}, y_0 = y_{01}, \rho = 0, \sigma = 1$). In the region 2 a rectangular SQL ($\rho = 0, \sigma \neq 1$) has the minimum energy. When b and γ increase, first, a first-order phase transition from a regular triangular SQL to a square one occurs, then a second-order phase transition from a square SQL to a rectangular one. The lines of the two phase transitions in the $b\gamma$ plane are close to each other and practically coincide with the boundary between the regions 1 and 2. Hence the region where a square SQL is energetically favored is not shown in Fig. 2. The dashed line in Fig. 1 corresponds to equal β for regular triangular SQL and TQL. This line coincides well with the

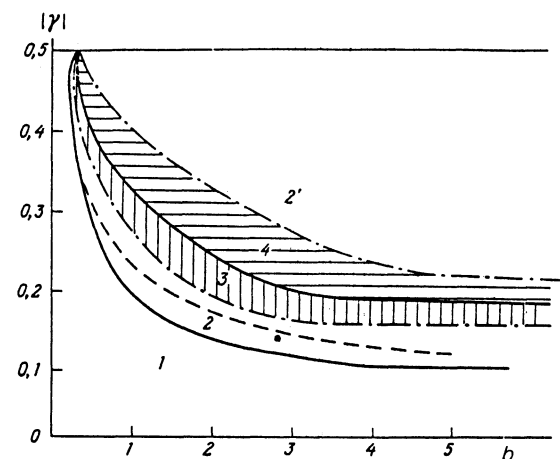


FIG. 2. Regions of energetic preference for different SQL and TQL types near H_{c2} . The region 1 corresponds to a regular triangular SQL, the regions 2 and 2' to a rectangular SQL, and in the regions 3 and 4 the values of β corresponding to a TQL and a rectangular SQL are equal to an accuracy of 10^{-3} .

boundary of the region (19) found in the Wigner–Seitz approximation. Of course, to get the β minimum in the regions 2, 3, 4, and 2', the Wigner–Seitz method is not good, since in these regions the rectangular SQL, which cannot be treated by this method, is energetically favorable. In the region 3 in the $b\gamma$ plane, to an accuracy of 10^{-3} , the values of β corresponding to a regular triangular TQL ($x_0 = x', y_0 = y', \rho = 1/4, \sigma = 3^{1/2}/4$) and a rectangular SQL become equal. To the same accuracy of 10^{-3} , the values of β in the region 4 are equal for a rectangular SQL and a square TQL ($x_0 = x', y_0 = y', \rho = 0, \sigma = \frac{1}{2}$). In the region 3 the TQL energy minimum with respect to ρ and σ corresponds to a regular triangular TQL, while in the region 4 it corresponds to a square TQL.

Let the smallest value of β for all TQL with different ρ and σ be β_{2m} , and let β_{1m} be the smallest value of β for different SQL. Numerical calculations have shown that $\beta_{2m} \geq \beta_{1m}$ holds for all b and γ . In region 2', as in region 2, a rectangular SQL is energetically favored. In this region the difference $\Delta\beta = \beta_{2m} - \beta_{1m}$ increases with increasing b and γ and, for example, for $b < 5$ satisfies the $\Delta\beta \leq 0.2$ condition. Parameter σ in SQL with $\beta = \beta_{1m}$ also increases with increasing b and γ , and, for instance, for $1.2 < b < 5$ and $\gamma = 0.5$ we have $\sigma \approx 2.5$. Thus, in the region 2' a rectangular SQL is, in fact, a set of vortex chains. The distance between the chains can be much larger than the distance between the vortices in one chain and increases with increasing b and γ . For a fixed and sufficiently large value of σ the value of β depends only weakly on ρ . This means that the lattice energy does not change much when vortex chains are displaced with respect to one another, if the distance between the chains remains constant. Note that, as a result of formation of such a lattice, transport properties in the mixed state could be highly anisotropic.

A regular triangular SQL becomes energetically unfavorable only for finite values of $\gamma > \gamma_{th}(b)$ (see Fig. 2). The existence of such a threshold in γ is easy to understand by virtue of symmetry considerations leading to the conditions (21) and (22) valid for all γ . It follows from Eqs. (21) and (22) that the point $\rho = \frac{1}{2}, \sigma = 3^{1/2}/2$ is an extremum point for $\beta(\rho, \sigma)$, even if $\gamma \neq 0$. Then, if for $\gamma = 0$ the function $\beta(\rho, \sigma)$ has a minimum, the corresponding lattice could be energetically unfavorable only for finite values of γ .

To conclude this section, we note a feature of the function β directly related to the fact that for a regular triangular TQL β is always larger than or equal to β_{1m} . Numerical calculations have shown that for $\rho = 1/4, \sigma = 3^{1/2}/4$ the function β is independent of x_0, y_0 . These values of ρ and σ correspond to a vortex lattice formed by regular triangular sublattices embedded into each other. When these sublattices coincide, we have a regular triangular TQL. Such an energy degeneracy occurs only near H_{c2} and is lifted with decreasing field (see Sec. 4). For $x_0 = x_{01}, y_0 = y_{01}$ we have a SQL with $\rho = 1/4, \sigma = 3^{1/2}/4$. Thus, the smallest value of β for a SQL cannot exceed β for a regular triangular TQL. Numerical calculations give the following expression for β ($\rho = 1/4, \sigma = 3^{1/2}/4$):

$$\beta = (1.338 + 9.035\gamma^4 + 3.109(1+2b)\gamma^2)(1+2\gamma^2)^{-2}. \quad (25)$$

This result agrees fairly well with Eq. (18b) found in the Wigner–Seitz approximation. Note that for a regular

triangular SQL numerical analysis has shown that $\beta(b, \gamma)$ is accurately described by Eq. (18a) found in the present approximation.

4. MAGNETIC PHASE TRANSITIONS

In this section we consider how the lattice structure varies with decreasing magnetic field H . As H decreases, the expression $(1 - H/H_{c2})/(H/\tilde{H} - 1)$ becomes of order unity, and we have to allow for superconducting seeds corresponding to the solutions of the linearized GL equations both for $H = H_{c2}$ and $H = \tilde{H}$. Let us seek the solution of the nonlinear GL equation in this field range in the form

$$\Psi_1 = R\varphi_0, \quad \Psi_2 = \gamma R\varphi_2 + F. \quad (26)$$

Here both F and φ_0 contain the wave functions of the zeroth Landau level. We limit ourselves in what follows by the case $D < C^2/(1+C)$. This case is of interest more often than the opposite one, since, due to approximate electron-hole symmetry near the Fermi surface, the coefficient $D = (K_2 - K_3)/2K_1$ is very small,¹⁹ and the coefficient C in UPT₃, according to Refs. 20 and 21, is approximately -0.29 .

Let the vortex lattices given by the functions $R\varphi_0$ and $\gamma R\varphi_2$ have the form (9). The lattice structure corresponding to F needs a special treatment. Substituting (26) into the GL-functional, we find for the free energy

$$\begin{aligned} f = & (H/H_{c2} - 1) (\langle |\varphi_0|^2 \rangle + \gamma^2 \langle |\varphi_2|^2 \rangle) |R|^2 + 0.5 \langle |\varphi_0|^4 \rangle |R|^4 + \gamma^2 (1 \\ & + 2b) |R|^4 \langle |\varphi_0|^2 |\varphi_2|^2 \rangle + 0.5 \gamma^4 \langle |\varphi_2|^2 \rangle |R|^4 + (H/\tilde{H} - 1) \langle |F|^2 \rangle + (1 \\ & + 2b) \langle |\varphi_0|^2 |F|^2 \rangle |R|^2 + 2(1+2b)\gamma |R|^2 \text{Re}(R \langle |\varphi_0|^2 \varphi_2 F^* \rangle) \\ & + 0.5 \langle |F|^4 \rangle \\ & + \gamma^2 \text{Re}(R^2 \langle (\varphi_2 F^*)^2 \rangle) + 2\gamma^2 |R|^2 \langle |\varphi_2|^2 |F|^2 \rangle \\ & + 2\gamma^3 |R|^2 \text{Re}(R \langle |\varphi_2|^2 \varphi_2 F^* \rangle) \\ & + 2\gamma \text{Re}(R \langle |F|^2 \varphi_2 F^* \rangle). \end{aligned} \quad (27)$$

The terms in (27) in which F is absent give the contribution to the free energy described by Eqs. (14) and (15). As H decreases, the sum of the terms quadratic in F ceases to be positive definite for a certain field value $H = H_{tr} < \tilde{H}$, where H_{tr} depends on the lattice structure.

For fields larger than H_{tr} the function F is small in comparison with Ψ_1 , and for $H \rightarrow H_{c2}$ we have $F/R \rightarrow 0$. Consider first the solution just in this field range, assuming $|\gamma| \ll 1$, which is justified by the inequality $|\gamma| < \frac{1}{2}$ following from Eqs. (2) and (5). The F -dependent terms in (27) are taken into account by perturbation theory. We neglect in (27) terms of the third and fourth order in F , as well as the terms proportional to γ^4, γ^3 , and write the resulting expression for f :

$$\begin{aligned} f = & f_0 + f_1; \\ f_0 = & (H/H_{c2} - 1) \langle |\varphi_0|^2 \rangle R^2 + 0.5 \langle |\varphi_0|^4 \rangle R^4 \\ & + \gamma^2 (1+2b) R^4 \langle |\varphi_0|^2 |\varphi_2|^2 \rangle, \\ f_1 = & \gamma^2 (H/H_{c2} - 1) \langle |\varphi_2|^2 \rangle R^2 + (H/\tilde{H} - 1) \langle |F|^2 \rangle \\ & + (1+2b) \langle |\varphi_0|^2 |F|^2 \rangle R^2 \\ & + 2(1+2b)\gamma R^3 \text{Re} \langle |\varphi_0|^2 \varphi_2 F^* \rangle. \end{aligned} \quad (28)$$

Let us treat f_1 as a perturbation, substituting into it the value $R = R_0$ obtained by minimization of f_0 :

$$R_0 = (1 - H/H_{c2}) / (\beta_0 \langle |\varphi_0|^2 \rangle); \langle |\varphi_0|^2 \rangle = (|\theta_{\text{even}}|^2 + |\theta_{\text{odd}}|^2) / 8\sigma)^{1/2}, \quad (29)$$

$$\beta_0 = \frac{\langle |\varphi_0|^4 \rangle + 2\gamma^2(1+2b)\langle |\varphi_0|^2 |\varphi_2|^2 \rangle}{\langle |\varphi_0|^2 \rangle^2}.$$

We get an expression for f accurate to terms of order γ^2 inclusive. Note that the term $\gamma^2 R^2(1+2b)\langle |\varphi_0|^2 |\varphi_2|^2 \rangle$ is taken into account in f_0 , since for fairly large b it might not be small even for small γ .

We are looking for F in the form

$$F = \sum_k S_k \exp(2\pi i k x / a_0 - 0.5((y - kb_0 \sin \alpha) / L_H)^2). \quad (30)$$

From the condition that f be a minimum with respect to the coefficients S_k , we find the following equation for S_k :

$$f = -(1 - H/H_{c2})^2 / (2\beta(H)), \quad \beta^{-1}(H) = (1 + 4\gamma^2) / \beta_0 + J(H), \quad (33)$$

$$J(H) = \frac{\gamma^2(1+2b)(\delta(|Q_1|^2 + |Q_2|^2) + \alpha_1|Q_2|^2 + \alpha_2|Q_1|^2 - 2\text{Re}(\alpha_3 Q_1^* Q_2))}{2\sigma^2 \beta_0^2 \langle |\varphi_0|^2 \rangle^2 ((\delta + \alpha_1)(\delta + \alpha_2) - |\alpha_3|^2)},$$

$$\delta = 2^{1/2} \beta_0 \langle |\varphi_0|^2 \rangle (1+2b)^{-1} (H/\bar{H} - 1) (1 - H/H_{c2})^{-1}.$$

The quantities Q_1 , Q_2 , α_1 , α_2 , α_3 , and β_0 depend on ρ , σ , θ_{even} and θ_{odd} (their formulae are given in Appendix).

The expressions (33) are valid until $0 < J(H)\beta_0 \ll 1$. It follows from them that in the fields close to H_{c2} ($H/\bar{H} - 1 \gg 1 - H/H_{c2}$) we can neglect the quantity

$$J(H) \sim \gamma^2 (1 - H/H_{c2}) / (H/\bar{H} - 1).$$

In this case the results of Sec. 3 are valid. If, however, we have $H/\bar{H} - 1 \sim 1 - H/H_{c2}$, then $J \sim \gamma^2$. In spite of their smallness, these corrections can affect the lattice structure, since, as seen from Sec. 3, the values of β_0 for different lattices are fairly close to one another. In the case of a SQL, the expression for $J(H)$ reduces to

$$J_{\text{SQL}}(H) = \frac{4\gamma^2(1+2b)^2(1 - H/H_{c2})\sigma^2}{\beta_0^3(2(H/\bar{H} - 1) + 2(1+2b)(1 - H/H_{c2})\beta_A/\beta_0)} \times \left[\left| \frac{\partial \beta_A}{\partial \sigma} \right|^2 + \left| \frac{\partial \beta_A}{\partial \rho} \right|^2 \right]. \quad (34)$$

Here $\beta_A = \beta_0(\gamma = 0)$ for a SQL. As is well-known, a square SQL and a regular triangular SQL correspond to the extrema of the function $\beta(\rho, \sigma)$, and, consequently, for them $J(H)$ vanishes. For arbitrary ρ and σ we have $J(H) \neq 0$, and $J(x, y)$ corresponds to a SQL coinciding with the component- Ψ_1 vortex lattice.

The expressions (33) have been analyzed numerically. By virtue of smallness of the coefficient D mentioned above, we have set $D = 0$. The lattices of the type (9) with arbitrary θ_{even} and θ_{odd} have been considered. Calculations have shown that $\beta(H)$ achieves its minimum only for the values of θ_{even} and θ_{odd} corresponding to a SQL or a TQL. In a certain parameter range the TQL can be rectangular, but, as the field decreases further, it always becomes regular triangular, for which $\theta_{\text{odd}}/\theta_{\text{even}} \approx 1.366(1 - i)$, and the coefficient ratio $s_{\text{even}}/s_{\text{odd}} \approx -1.366(1 + i)$ does not depend on H . Such values of s_{even} and s_{odd} can be found from (10), if we set $x_0 = 5a_0/8$, $y_0 = -4b_0 \sin \alpha / 3$. The position of the zeros of the functions Ψ_1 and F in a regular triangular TQL is

$$2^{1/2} (H/\bar{H} - 1) S_k + (1+2b) R_0^2 \times \sum_{nm} S_{m+k} c_{n+k} c_{n+m+k} \exp(-\pi\sigma(n^2 + m^2)) = (1+2b) \gamma R_0^3 \sum_{nm} c_{m+k} c_{n+k} c_{n+m+k} (0.5 - \pi\sigma(n-m)^2) \times \exp(-\pi\sigma(n^2 + m^2)). \quad (31)$$

The coefficients c_n are defined in (9). The solution of (31) has the form

$$S_k = \exp(i\pi\rho k(k-1)) s_k = \begin{cases} s_{\text{even}} & \exp(i\pi\rho k(k-1)), \\ s_{\text{odd}} & \exp(i\pi\rho k(k-1)). \end{cases} \quad (32)$$

The upper expression is valid for even k , and the lower for odd k . Substituting (32) into (31), we can find s_{even} and s_{odd} . Using this solution, we get f :

shown in Fig. 3 The zeros of the function F are located at the intersections of the medians of the triangles, the vertices of which contain the Ψ_1 vortices. Before discussing at length the results of numerical calculations, let us generalize the suggested approach to the case of fields $H < H_{tr}$, when the sum of the terms quadratic in F in Eq. (27) ceases to be positive definite. For fields below H_{tr} the function F is not small in comparison with Ψ_1 , and, in order to find it, it is necessary to allow for terms of third and fourth order in F in the expression for the free energy. This can be done relatively simply only in those cases when the component- Ψ_1 lattice is a SQL or a regular triangular TQL.

To solve this problem, let us use the perturbation theory in γ . Without the terms proportional to γ , γ^2 , γ^3 , and γ^4 , the free energy (27) takes the form

$$f = (H/H_{c2} - 1) \langle |\varphi_0|^2 \rangle R^2 + 0.5 \langle |\varphi_0|^4 \rangle R^4 + (H/\bar{H} - 1) \langle |F|^2 \rangle + (1+2b) \langle |\varphi_0|^2 |F|^2 \rangle R^2 + 0.5 \langle |F|^4 \rangle. \quad (35)$$

The absolute value of the function F , corresponding to the free-energy minimum, should have the same periodicity

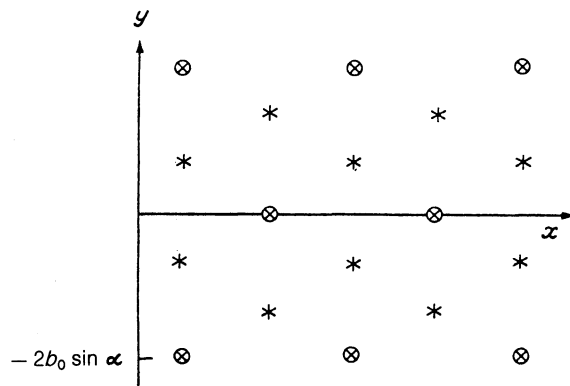


FIG. 3. The location of the zeros of the functions Ψ_1 and F for a regular triangular TQL: \otimes is the function- Ψ_1 zero, and $*$ is the function- F zero.

as the function $|\varphi_0|$. The nonzero component $\Psi_2 = F$ appears against the background of the already existing component $\Psi_1 = R\varphi_0$ only in the fields $H < H_{tr}$, where H_{tr} is defined by the equation

$$(H_{tr}/\bar{H}-1) + (1+2b)(1-H_{tr}/H_{c2})\langle|\varphi_0|^2\rangle \times \frac{\langle|\varphi_0|^2|F|^2\rangle}{\langle|F|^2\rangle\langle|\varphi_0|^4\rangle} = 0. \quad (36)$$

Note that H_{tr} exists not for all $b > 0$, and only for b smaller than a certain critical value.

In the case when φ_0 corresponds to a SQL, we seek F in the form

$$F(x, y, \tilde{x}, \tilde{y}) = s\varphi_0(x-\tilde{x}, y-\tilde{y})\exp(i\tilde{y}x/L_H^2). \quad (37)$$

Here (\tilde{x}, \tilde{y}) is the vector, by which the vortex lattice corresponding to F is displaced with respect to the lattice φ_0 . In Eq. (35) only the quantity $\langle|\varphi_0|^2|F|^2\rangle$ depends on \tilde{x}, \tilde{y} . Minimizing it with respect to these variables, we can find \tilde{x}_m, \tilde{y}_m corresponding to the Ψ_2 lattice and, consequently, the largest possible field H_{tr} for the given function φ_0 (with definite ρ and σ). For a regular triangular SQL

$$\tilde{x}_m = 0, \quad \tilde{y}_m = -2b_0 \sin \alpha/3,$$

and the transition field H_{tr} has the form

$$H_{tr} = \frac{H_{c2}}{1 + (H_{c2}/\bar{H}-1)/(0.21-1.58b)}. \quad (38)$$

For a square SQL $\tilde{x}_m = a_0/2, \tilde{y}_m = -a_0/2$. For a rectangular SQL with a sufficiently large parameter $\sigma > 2$ the quantity $\langle|\varphi_0|^2|F|^2\rangle$ has a very weak \tilde{x} -dependence, and $\tilde{y}_m = -b_0/2$.

For a regular triangular TQL of the component Ψ_1 F is chosen as a function describing a lattice with $\rho = 0.25$, $\sigma = 3^{1/2}/4$, and a flux through the unit cell equal to $2\Phi_0$ displaced by the vector (\tilde{x}, \tilde{y}) :

$$F = R_F G_F(x, y) = \sum_n R_F S_n \exp(2\pi i n(x-\tilde{x})/a_0 - 0.5((y-\tilde{y}-nb_0 \sin \alpha)/L_H)^2) \exp(i\tilde{y}x/L_H^2). \quad (39)$$

The coefficients S_n have the form (32). Substituting $\tilde{R}_F^2 = R_F^2 \langle|G_F|^2\rangle$ in (35) and taking into account that the relation $\langle|G_F|^4\rangle/\langle|G_F|^2\rangle^2$ for $\rho = 0.25, \sigma = 3^{1/2}/4$ does not depend on s_{even} and s_{odd} (see Sec. 3), we make sure that the minimum of the f function $\langle|\varphi_0|^2|G_F|^2\rangle/(\langle|\varphi_0|^2\rangle\langle|G_F|^2\rangle)$ corresponds to the minimum of the function f with respect to $\tilde{x}, \tilde{y}, s_{\text{even}}$ and s_{odd} . The following values of the variables, for which this minimum is realized, have been found numerically: $\tilde{x} = 0, \tilde{y} = 0, s_{\text{even}}/s_{\text{odd}} = -1.366(1+i)$. It follows from (36) that the field H_{tr} is largest for these values.

Let us now analyze the terms in γ and γ^2 in the expression (27) for the free energy. For a regular triangular TQL of the component Ψ_1 , the form of the function F found for $\gamma = 0$ coincides with the induced solution for F for $\gamma \neq 0$ in the field range $\bar{H} < H < H_{c2}$ considered above. This allows to assume that in the whole range of fields H sufficiently close to H_{c2} the solution (Ψ_1, Ψ_2) , in this case, can be sought in the form (26), where φ_0 and φ_2 are found from Eq. (9), the function F from Eq. (39), and $\tilde{x} = \tilde{y} = 0, \theta_{\text{odd}}/\theta_{\text{even}} = 1.366(1-i), s_{\text{even}}/s_{\text{odd}} = -1.366(1+i)$. We substitute this solution into (27), neglecting the terms in γ^3 and γ^4 . Making the change $R_F = R\tau$ and finding the minimum of f with respect to R , we get

$$f = -0.5(1-H/H_{c2})^2/\beta(H, \tau), \quad (40)$$

$$\beta(H, \tau) = \frac{A_2 + B_2|\tau|^4 + 2d_1|\tau|^2 + 2\text{Re}(2\gamma(1+2b)d_2\tau + 2\gamma^2 d_3\tau^2 + 2\gamma|\tau|^2 d_4\tau)}{(A_1 + B_1|\tau|^2(1-H/\bar{H})/(1-H/H_{c2}))^2},$$

if

$$(1-H/H_{c2})A_1 + B_1|\tau|^2(1-H/\bar{H}) > 0;$$

$$f = 0, \text{ for } (1-H/H_{c2})A_1 + B_1|\tau|^2(1-H/\bar{H}) \leq 0.$$

Here

$$d_1 = (1+2b)\langle|\varphi_0|^2|G_F|^2\rangle + 2\gamma^2\langle|\varphi_2|^2|G_F|^2\rangle,$$

$$d_2 = \langle|\varphi_0|^2\varphi_2^*G_F\rangle,$$

$$d_3 = 0.5\langle\varphi_2^*G_F\rangle, \quad d_4 = \langle|G_F|^2G_F\varphi_2^*\rangle,$$

$$B_1 = \langle|G_F|^2\rangle = (|s_{\text{even}}|^2 + |s_{\text{odd}}|^2)/(8\sigma)^{1/2},$$

$$B_2 = \langle|G_F|^4\rangle, \quad A_1 = \langle|\varphi_0|^2\rangle + 2\gamma^2\langle|\varphi_2|^2\rangle$$

$$= (1+2\gamma^2)(|\theta_{\text{even}}|^2 + |\theta_{\text{odd}}|^2)/(8\sigma)^{1/2},$$

$$A_2 = \langle|\varphi_0|^4\rangle + 2\gamma^2(1+2b)\langle|\varphi_0|^2|\varphi_2|^2\rangle.$$

The formulae of the averaged functions are given in the Appendix.

It is convenient to find the minimum of $\beta(H, \tau)$ numerically. The function $\beta_{\text{min}}(H)$ in the range $\bar{H} < H < H_{c2}$ is given by Eq. (33) for a regular triangular TQL in the quadratic approximation in γ .

Let us consider now the case of the component- Ψ_1 SQL.

The lattice corresponding to F for $\gamma = 0$ is displaced by the vector $(\tilde{x}_m, \tilde{y}_m)$ with respect to the Ψ_1 lattice. Therefore the averages

$$\langle|\varphi_0|^2\varphi_2^*F^*\rangle, \quad \langle|\varphi_2|^2\varphi_2^*F^*\rangle, \quad \langle|F|^2\varphi_2^*F^*\rangle,$$

arising in Eq. (27) in the next orders in γ reduce to zero. This is related to various transformation properties of the functions φ_0, φ_2 , and F under translations through lattice vectors. For F these properties can be found from (37):

$$F(x+a_0, y) = F(x, y)\exp(2\pi i\tilde{y}_m/(b_0 \sin \alpha)),$$

$$F(x+b_0 \cos \alpha, y-b_0 \sin \alpha)$$

$$= F(x, y)\exp(-2\pi ix/a_0 + 2\pi i\tilde{x}_m/a_0 + 2\pi i\tilde{y}_m \text{ctg} \alpha/a_0). \quad (41)$$

Performing these transformations of the integration variables in the expression $\langle|\varphi_0|^2\varphi_2^*F^*\rangle$, we find, for example,

$$\langle|\varphi_0|^2\varphi_2^*F^*\rangle = \exp(-2\pi i\tilde{y}_m/(b_0 \sin \alpha))\langle|\varphi_0|^2\varphi_2^*F^*\rangle.$$

Hence, for $\tilde{y}_m \neq nb_0 \sin \alpha$, it follows that $\langle|\varphi_0|^2\varphi_2^*F^*\rangle = 0$. Using such relations, it is possible to prove that all the averages mentioned above vanish, if F does not coincide with φ_0 .

Allowing for these properties of the solution for $\gamma = 0$ and taking into account that for $\gamma \neq 0$ we have $F = s\varphi_0$ in the field range $\tilde{H} < H < H_{c2}$, we look for Ψ_1 and Ψ_2 in the form

$$\Psi_1 = R\varphi_0(x, y), \quad (42)$$

$$\Psi_2 = \gamma R\varphi_2(x, y) + s\varphi_0(x, y) + V\varphi_0(x - \tilde{x}_m, y - \tilde{y}_m) \exp(i\tilde{y}_m x / L_H^2).$$

$$V = |V| \exp(i\delta_V).$$

Substituting (42) into (27), we find in the approximation quadratic in γ

$$\begin{aligned} f &= f_0 + f_1, \\ f_0 &= (H/H_{c2} - 1) \langle |\varphi_0|^2 \rangle R^2 + 0.5 \langle |\varphi_0|^4 \rangle \\ &\quad + 2\gamma^2 (1 + 2b) \langle |\varphi_0|^2 |\varphi_2|^2 \rangle R^4 \\ &\quad + (H/\tilde{H} - 1) |V|^2 \langle |\varphi_0|^2 \rangle + (1 + 2b) \langle |\varphi_0|^2 |G|^2 \rangle R^2 |V|^2 \\ &\quad + 0.5 |V|^4 \langle |\varphi_0|^4 \rangle, \\ f_1 &= (H/H_{c2} - 1) \gamma^2 \langle |\varphi_2|^2 \rangle R^2 + 2\gamma^2 |V|^2 \tilde{R}^2 \langle |\varphi_2|^2 |G|^2 \rangle \\ &\quad + \gamma^2 R^2 \operatorname{Re} \langle \varphi_2^* G^2 V^{*2} \rangle \\ &\quad + |s|^2 ((H/\tilde{H} - 1) \langle |\varphi_0|^2 \rangle + R^2 (1 + 2b) \langle |\varphi_0|^4 \rangle \\ &\quad + 2|V|^2 \langle |G|^2 |\varphi_0|^2 \rangle) \\ &\quad + 2\gamma (1 + 2b) R^2 \operatorname{Re} \langle s \langle |\varphi_0|^2 \varphi_2^* \varphi_0 \rangle + 4\gamma R |V|^2 \operatorname{Re} \langle s \langle |G|^2 \varphi_2^* \varphi_0 \rangle \rangle \\ &\quad + 2\gamma R \operatorname{Re} \langle s V^{*2} \langle G^2 \varphi_0 \varphi_2 \rangle \rangle. \end{aligned} \quad (43)$$

Here $G(x, y) = \varphi_0(x - \tilde{x}_m, y - \tilde{y}_m) \exp(i\tilde{y}_m x / L_H^2)$. Since $s \sim \gamma$, we will treat a part of the free energy f_1 as a perturbation, substituting into it the values of $|V_m|$ and R_m found from the minimization of f_0 . For $H > H_{tr}$, we have

$$V_m = 0, \quad R_m^2 = \chi(1 - H/H_{c2}) = (1 - H/H_{c2}) / (\beta_0 \langle |\varphi_0|^2 \rangle). \quad (44a)$$

For $H < H_{tr}$, then

$$\begin{aligned} R_m^2 &= \chi(1 - H/H_{c2}) \\ &= \frac{\langle |\varphi_0|^2 \rangle ((1 - H/\tilde{H})(1 + 2b)Z - (1 - H/H_{c2})\beta_A \langle |\varphi_0|^2 \rangle)}{(1 + 2b)^2 Z^2 - \langle |\varphi_0|^2 \rangle^4 \beta_A \beta_0}, \end{aligned} \quad (44b)$$

$$\begin{aligned} |V_m|^2 &= \omega(1 - H/H_{c2}) \\ &= \frac{\langle |\varphi_0|^2 \rangle ((1 - H/H_{c2})(1 + 2b)Z - (1 - H/\tilde{H})\beta_0 \langle |\varphi_0|^2 \rangle)}{(1 + 2b)^2 Z^2 - \langle |\varphi_0|^2 \rangle^4 \beta_A \beta_0}, \end{aligned}$$

$$H_{tr} = H_{c2} \left[1 + \frac{H_{c2}/\tilde{H} - 1}{1 - (1 + 2b)Z / (\beta_0 \langle |\varphi_0|^2 \rangle)} \right]^{-1} \quad (45)$$

Here $Z = \langle |\varphi_0|^2 |G|^2 \rangle$, β_0 is defined by (29), and $\beta_A = \beta_0$ ($\gamma = 0$). Note that the term $2\gamma^2(1 + 2b) \langle |\varphi_0|^2 |\varphi_2|^2 \rangle R^4$ may not be small and so is included in f_0 , similar to (28). Finding now the minimum of f with respect to s , we get the following expression for the energy:

$$\begin{aligned} f &= -0.5(1 - H/H_{c2})^2 / \beta(H), \\ \beta^{-1}(H) &= (2/\sigma)^{1/2} \chi(1 + 2\gamma^2) - \chi^2 \beta_0 / \sigma \\ &\quad + (2/\sigma)^{1/2} (1 - H/\tilde{H}) \omega / (1 - H/H_{c2}) \\ &\quad - \beta_A \omega^2 / \sigma - \chi \omega (2(1 + 2b)Z + \gamma^2 \Gamma) \\ &\quad - 2\chi \omega \gamma^2 \operatorname{Re} \langle \varphi_2^* G^2 \rangle \exp(-2i\delta_V) \\ &\quad + \frac{\gamma^2 \chi | (1 + 2b) \chi \rho_1 + 2\omega \rho_2 - 2\omega \sigma^{1/2} \exp(2i\delta_V) \langle G^2 \varphi_0^* \varphi_2 \rangle |^2}{(2\sigma)^{1/2} (H/\tilde{H} - 1) / (1 - H/H_{c2}) + (1 + 2b) \chi \beta_A + 4\sigma Z \omega}, \end{aligned} \quad (46)$$

$$\Gamma = 4 \langle |\varphi_2|^2 |G|^2 \rangle, \quad \rho_1 = -2\sigma^{1/2} \langle |\varphi_0|^2 \varphi_2 \varphi_0^* \rangle,$$

$$\rho_2 = -2\sigma^{1/2} \langle |G|^2 \varphi_2 \varphi_0^* \rangle.$$

The expressions for the averages Z , Γ , ρ_1 , and ρ_2 are given in Appendix. The coordinates \tilde{x}_m and \tilde{y}_m are determined here by numerical minimization of Z . For the case of a regular triangular Ψ_1 lattice the averages $\langle \varphi_2^2 G^* \rangle$ and $\langle G^2 \varphi_0^* \varphi_2^* \rangle$ reduce to zero. If the Ψ_1 lattice is rectangular, these averages do not vanish, but the contribution of the relevant terms in (46) is small, and the free energy depends weakly on δ_V .

Note that since the function $G(x, y)$ transforms under translations like the function F in (37), the absolute value of the component Ψ_2 for $\gamma \neq 0$ can be periodic in the x, y plane with periods other than those of $|\varphi_0|$. The unit cell of such a lattice can contain several single-quantum vortices of the component Ψ_1 , and, consequently, the magnetic flux enclosed by the cell can be larger than Φ_0 . Thus, for example, if the Ψ_1 lattice is rectangular ($\rho = 0$), then $\tilde{y}_m = -b_0/2$, $\tilde{x}_m = a_0/2$ and $|\Psi_2|$ has the following properties:

$$|\Psi_2(x \pm a_0, y \mp b_0)| = |\Psi_2(x, y)|.$$

In this case the unit cell encloses two quanta of magnetic flux. The lattices of the type (42) are nonsingular for $H < H_{tr}$ (and we have $V \neq 0$).

We now present the results of numerical analysis of Eqs. (33), (40), and (46) for various values of the parameters b and γ . In Figs. 4–6 we have shown in the Hb plane the regions in which various lattice types are energetically preferred for fixed γ values. From the above-mentioned condition $D = 0$, as well as from Eqs. (2) and (5), it follows that the parameter $\varepsilon = C/(1 + C)$ should satisfy the inequality $|\varepsilon| < 0.5$. This being the case, we have $|\gamma| < \sqrt{1.5} - 1 \approx 0.225$.

In the case $\gamma = 0$ (Fig. 4a) we have $\tilde{H} = H_{c2}$, and, consequently there is no field range where the results of Sec. 3 are valid. The quantity β does not depend on H [see (40) and (46)]. The optimization of Eq. (46) for β with respect to ρ and σ and comparison with a TQL [Eq. (40)] show that for all $b > 0.45$ a regular triangular singular SQL has the lowest energy (in this case either Ψ_1 or Ψ_2 vanishes). A nonsingular rectangular SQL corresponds to $b < 0.45$ (see Fig. 4a). For $b = 0$ its energy becomes equal to the energy of a regular triangular TQL.

Let us explain these results. A nonsingular lattice with given ρ and σ is more favorable than a singular one with the same ρ and σ for $b < b'$, where

$$b'(\rho, \sigma) = 0.5 (\langle |\varphi_0|^4 \rangle / \langle |\varphi_0|^2 |F|^2 \rangle - 1).$$

The function F is given by Eq. (37). As σ increases the quantity b' grows and for $\sigma \rightarrow \infty$ we have $b' \sim \exp(\pi\sigma/4)$. For $b < b'(\rho, \sigma)$ the value of $\beta(\rho, \sigma)$ corresponding to a SQL decreases with decreasing b and for a certain $\tilde{b}(\rho, \sigma)$ becomes smaller than the value of β for a singular regular triangular SQL ($\rho = \frac{1}{2}, \sigma = 3^{1/2}/2$). For certain values of ρ and σ this b could be larger than the threshold value $b'(\rho = \frac{1}{2}, \sigma = 3^{1/2}/2) = 0.13$. As mentioned above, the largest \tilde{b} equals 0.45 (for $\sigma_m \approx 3.7$). With decreasing b , the value of σ_m corresponding to the most favored SQL falls off, and for $b = 0$ we have $\sigma_m \approx 1.73$.

For $\gamma \neq 0$ the parameter β becomes a function of H , and as the magnetic field decreases phase transitions accompanied by changes in the vortex lattice structure occur. For $H \rightarrow H_{c2}$ the lattice types described in Sec. 3 are realized. The

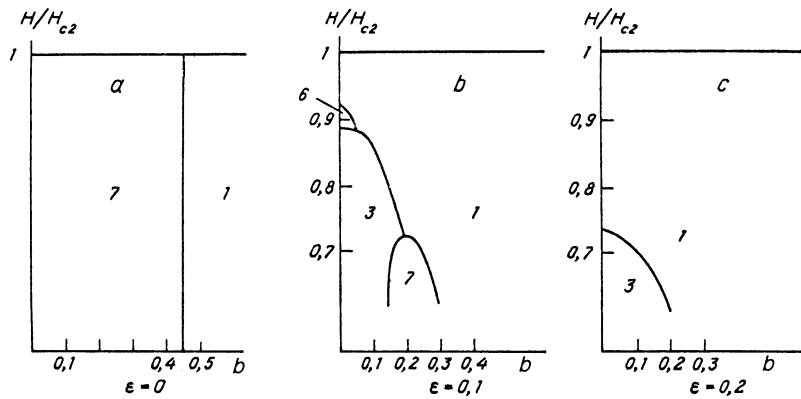


FIG. 4. Phase diagrams for small ϵ . The region 1 corresponds to a regular triangular SQL, the region 3 to a regular triangular TQL, and the regions 6 and 7 to a nonsingular lattice of the type (42) with $\rho = 0$, $\sigma = 1$ and $\rho = 0$, $\sigma \neq 1$ respectively.

label 1 in Figs. 4–6 denotes the regions, in which a singular regular triangular SQL is energetically favored, and the figures 2 and 2' the regions of a singular rectangular SQL. When the field H falls off, the energy degeneracy with respect to the sublattice displacement taking place in the lattice with $\rho = 1/4$, $\sigma = 3^{1/2}/4$ for $H \rightarrow H_{c2}$ (see Sec. 3) is lifted. The minimum with respect to x_0 and y_0 corresponds to a regular triangular TQL. This fact enlarges the region 3 where a regular triangular TQL is favored (Figs. 5 and 6). In this case a transition to a TQL may be obtained even for $\tilde{H} < H < H_{c2}$ if we use Eq. (33). For sufficiently large values of b and ϵ the transition from a rectangular SQL to a rectangular TQL (the region 5 in Fig. 6) occurs first, and then the transition to a regular triangular TQL. For parameter values corresponding to the regions 3 and 4 in Fig. 2 the field of the SQL–TQL phase transition is very close to H_{c2} and its determination is not quite correct due to the approximations used ($\kappa \gg 1, \gamma \ll 1$).

For $\epsilon \lesssim 0.23$ the region 3 is divided into two parts corresponding to large and small b (cf. Figs. 4 and 5). For small b the transition to a TQL occurs in fields $H < \tilde{H}$, and in order to describe it we should use Eqs. (40) and (46). Of course, we neither allow for possible deviations of the TQL structure from a regular triangular lattice nor consider the case of arbitrary parameters θ_{even} and θ_{odd} .

For $\epsilon \lesssim 0.1$ and $b < 0.4$ the phase diagram becomes more complicated (Fig. 4b). Thus, for example, for $\epsilon = 0.1$ and $b < 0.05$ a narrow region 6 arises in which a nonsingular lattice of the form (42) with $\rho = 0$, $\sigma = 1$ corresponds to the

energy minimum. Furthermore, for $b > 0.05$ a transition to a nonsingular rectangular Ψ_1 lattice also given by Eq. (42) (the region 7 in Fig. 4b) may occur with decreasing field. The region 7 becomes larger as ϵ decreases and the region 3 becomes more narrow until it disappears completely as $\epsilon \rightarrow 0$ (Fig. 4a). The phase transition from a singular triangular SQL to a nonsingular structure of the type (42) with $\rho = 0.5$, $\sigma = 3^{1/2}/2$ is not realized since in the fields higher than H_{tr} ($\rho = 1/2, \sigma = 3^{1/2}/2$) [see (38)] either a TQL becomes energetically favored or a nonsingular lattice of the form (42) with $\rho = 0$.

Note that calculations have been carried out also for such H fields, for which the condition $(1 - H/H_{c2}) \ll 1$ does not already hold. It has been shown in Ref. 16 that in the case of ordinary superconductors the approach used near H_{c2} is applicable for fields $H \gtrsim 0.4H_{c2}$. Superconductors with a two-component order parameter are characterized by the existence of two close maxima H_m : \tilde{H} and H_{c2} (see Secs. 1 and 2). The other H_n , as in ordinary superconductors, are substantially smaller than H_{c2} . Therefore we can hope that the results found above are valid even when the inequality $(1 - H/H_{c2}) \ll 1$ does not hold.

All phase transitions between different types of vortex lattices (Figs. 4–6) are first-order phase transitions.

Let us determine the symmetry groups of these phases, limiting ourselves to the case in which the order parameter corresponds to the two-dimensional representation E_1 of the group D_6 . Then, for example, for singlet pairing the superconducting order parameter has the form

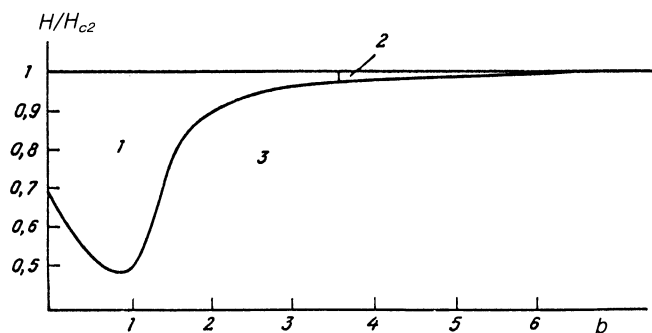


FIG. 5. The phase diagram for $\epsilon = 0.23$ corresponding to the region of a regular triangular TQL (3) divided into two parts for large and small b : the region 1 corresponds to a regular triangular SQL and the region 2 to a rectangular SQL.

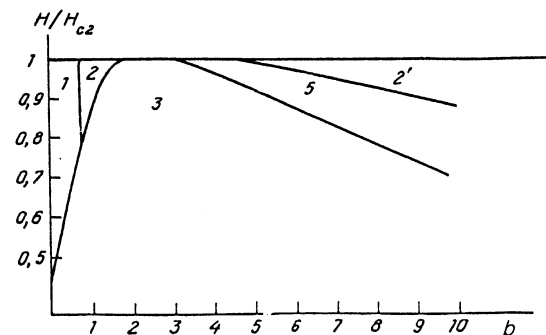


FIG. 6. The phase diagram for the largest possible $\epsilon = 0.5$ ($D = 0$): the region 1 corresponds to a regular triangular SQL, the region 3 to a regular triangular TQL, the region 5 to a rectangular TQL, and the regions 2 and 2' to a rectangular SQL.

$$\Delta_{\alpha\beta} = i\delta^{\alpha\beta}\Delta(k, r) = i\delta^{\alpha\beta}(\eta_1 k_x/k_x + \eta_2 k_y/k_y),$$

where (η_1, η_2) transform like the components of a two-dimensional vector in the x, y plane.¹⁹ The symmetry group of $\Delta(\mathbf{k}, \mathbf{r})$ for a regular triangular SQL (the region 1 in Figs. 2, 4–6) includes magnetic translations T_{e_1}, T_{e_2} through the vectors $e_1 = (a_0, 0)$ and $e_2 = (b_0 \cos \alpha, -b_0 \sin \alpha)$, magnetic rotations through the angle $\pi/3$ ($L_{\pi/3}$) around the axes parallel to z and passing through the zero points of the component Ψ_1 in the xy plane, reflections σ_z in the plane perpendicular to H , and transformations RU_2 [R is time reversal and U_2 denotes rotations through the angle π around the axes lying in the (x, y) plane]:

$$G_1 = \{T_{e_1}, T_{e_2}, -\sigma_z, RU_{2x}, RU_{2y}, L_{\pi/3}\}, \quad (47)$$

where U_{2x}, U_{2y} , and $L_{\pi/3}$ are the rotations around the axes passing through the point $(0; -(3^{1/2}/4)a_0)$. For a rectangular SQL (regions 2 and 2' in the figures) the symmetry group has the form

$$G_2 = \{T_{e_1}, T_{e_2}, -\sigma_z, -RU_{2x}, RU_{2y}, -L_{\pi}\}. \quad (48)$$

The rotations U_{2x}, U_{2y} , and L_{π} are around the axes passing through the origin. For a square SQL we have

$$G_{2C} = \{T_{e_1}, T_{e_2}, -\sigma_z, -RU_{2x}, RU_{2y}, -iL_{\pi/2}\}. \quad (49)$$

In the case of a regular triangular TQL (the region 3 in the figures) we have

$$G_3 = \{T_{e_1}, T_{2e_2}, -\sigma_z, -RU_{2x}, RU_{2y}, \exp(i\pi/3)L_{\pi/3}\}, \quad (50)$$

and the rotation axes pass through the point $(5a_0/8, 0)$. For square and rectangular TQL (regions 4 and 5)

$$G_4 = \{T_{e_1}, T_{2e_2}, -\sigma_z, -RU_{2x}, RU_{2y}, iL_{\pi/2}\}, \quad (51)$$

$$G_5 = \{T_{e_1}, T_{2e_2}, -\sigma_z, -RU_{2x}, RU_{2y}, -L_{\pi}\}. \quad (52)$$

where $L_{\pi}, L_{\pi/2}, U_{2x}$, and U_{2y} are the rotations around the axes passing through the point $(a_0/2, 0)$.

For nonsingular lattices of single-quantum vortices of the form (42) with two quanta of magnetic flux per unit cell symmetry properties substantially depend on the phase δ_V of the complex value V . For $V \neq 0$, in the case of square and rectangular Ψ_1 lattices (regions 6 and 7 in Fig. 6) the symmetry of $\Delta(\mathbf{k}, \mathbf{r})$ with respect to the transformations RU_2, L_{π} and $L_{\pi/2}$ is broken, but the symmetry with respect to combined rotations of the form $RU_{2x}L_{\pi}$ and to combinations of rotations and translations can be conserved. For $\gamma = 0$, the free energy does not depend on δ_V . In this case the lattice symmetry group in the region 7 of Fig. 4a is

$$G_7 = \{T_{e_1+e_2}, T_{e_1-e_2}, -\sigma_z, -T_{e_1}L_{\pi}, -T_{e_2}L_{\pi}, RU_{2y}, RU_{2x}L_{\pi}, -T_{e_1}RU_{2x}, -T_{e_2}RU_{2x}\} \text{ for } \delta_V = 0, \pi; \quad (53)$$

$$G_7 = \{T_{e_1+e_2}, T_{e_1-e_2}, -\sigma_z, -T_{e_1}L_{\pi}, -T_{e_2}L_{\pi}, -RU_{2x}, -RU_{2y}L_{\pi}, T_{e_1}RU_{2y}, T_{e_2}RU_{2y}\} \text{ for } \delta_V = \pm\pi/2, \quad (54)$$

$$G_7 = \{T_{e_1+e_2}, T_{e_1-e_2}, -\sigma_z, -T_{e_1}L_{\pi}, -T_{e_2}L_{\pi}\} \text{ for all other values of } \delta_V. \quad (55)$$

Here the rotations are performed around the axes passing through the origin. For $\gamma \neq 0$ in the case of a rectangular Ψ_1 lattice the energy degeneracy in δ_V is lifted, and the minimum of the energy (46) is achieved for $\delta_V = \pm\pi/2$, if

$\sigma > 1$. The lattice symmetry group in the region 7 in Fig. 4b thus has the form (54), if the period of the function $|\Psi_1|$ in y is larger than that in x (i.e., $\sigma = b_0/a_0 > 1$).

If the Ψ_1 lattice is square (the region 6 in Fig. 4b), the free energy is independent of δ_V also for $\gamma \neq 0$, since the averages $\langle \varphi_2^2 G^{*2} \rangle$, $\langle |\varphi_0|^2 \varphi_2 \varphi_0^* \rangle$, and $\langle |G|^2 \varphi_2 \varphi_0^* \rangle$ reduce to zero. The symmetry group G_6 of the order parameter $\Delta(\mathbf{k}, \mathbf{r})$ coincides in this case with G_7 for $\delta_V \neq \pm\pi/4, 3\pi/4$, and $5\pi/4$. For $\delta_V = \pi/4, 5\pi/4$

$$G_6 = \{T_{e_1+e_2}, T_{e_1-e_2}, -\sigma_z, -T_{e_1}L_{\pi}, -T_{e_2}L_{\pi}, iRU_{2x}L_{\pi/2}\}. \quad (56)$$

For $\delta_V = -\pi/4, 3\pi/4$

$$G_6 = \{T_{e_1+e_2}, T_{e_1-e_2}, -\sigma_z, -T_{e_1}L_{\pi}, -T_{e_2}L_{\pi}, -iRU_{2y}L_{\pi/2}\}. \quad (57)$$

To find δ_V in such a lattice, it is necessary to allow for higher-order terms in Ψ_1 and Ψ_2 in the free energy expansion.

5. CONCLUSION

Thus, using the formulae (33), (40), and (46), we arrive at the conclusion that near H_{c2} there are various phase transitions for different values of the parameters $\varepsilon = C/(1+C)$ and b . For small $b \leq 0.4$ and $\varepsilon \leq 0.1$ this may be a transition from a regular triangular SQL for high fields to a nonsingular lattice formed by single-quantum Ψ_1 vortices (Fig. 4b) whose existence has been suggested in Refs. 7 and 9. When the field decreases, a SQL–TQL transition occurs in the widest possible parameter range. This qualitatively agrees with the direct numerical solution of the GL equations in Ref. 10, but quantitative comparison is impossible, since the values of the parameters b and C , for which calculations have been carried out, are not indicated in Ref. 10. Experiments²⁰ on H_{c1} and H_{c2} measurement have yielded $b \approx 0.17$ and $C \approx -0.29$. For such b and C the SQL–TQL transition occurs for $H \approx 0.57H_{c2}$, which is fairly close to the experimental value.^{13–15}

For the parameters b and C corresponding to the regions 3, 4 and 2' in Fig. 2, the TQL and rectangular SQL energies are very close to each other, and a slight decrease in the field shows that a TQL is more favored. Thus, the estimates made in Ref. 8 by the Wigner–Seitz method are qualitatively correct, $\sin \varphi$ they indicate the TQL existence near H_{c2} . For $\kappa \gg 1$, as already discussed in Sec. 3, single-quantum vortices are energetically favored near H_{c1} . This means that besides the considered transition to a TQL for decreasing H a transition from a TQL to a single-quantum vortex lattice should occur⁸ in the field range, for which the inter-vortex distance satisfies the condition $\xi \ll d < \lambda$.

When this paper was ready for publication, I learned the results of Refs. 22 and 23. In Ref. 23 phase transitions in exotic superconductors are studied on the basis of further development of the symmetry analysis proposed in Ref. 11. For the GL functional of the form (1) and in the case $\mathbf{H} \parallel z$ and $b > 0$ considered above only one phase transition was obtained in Ref. 23: from a single-quantum hexagonal vortex lattice to a lattice with tripled number of flux quanta per unit cell. The authors treat only regular triangular lattices of component- Ψ_1 single-quantum vortices (tripling is connected with Ψ_2), and allow neither for single-quantum Ψ_1 lattices with arbitrary ρ and σ (including rectangular ones) nor for two-quantum Ψ_1 lattices. As follows from the above

analysis, allowance for such possibilities is important and leads for $b > 0$ and $\mathbf{H} \parallel z$ to a phase transition pattern, which differs qualitatively from that found in Ref. 23.

Furthermore, a singular-nonsingular vortex lattice transition for $\mathbf{H} \parallel z$ has been discussed in Refs. 22 and 23. Note that though the GL equation solutions differ substantially for $\mathbf{H} \parallel z$ and $\mathbf{H} \perp z$, in the latter case it may also prove important to allow for changes in ρ and σ in a single-quantum vortex lattice and TQL formation.

I would like to thank Yu. S. Barash for supervision and help. I am grateful to M. E. Zhitomirskii for acquainting me with the results of Ref. 23 before its publication, and I thank G. E. Volovik for helpful discussions.

APPENDIX

This Appendix includes some formulae used to calculate the quantities entering into Eqs. (33), (40), and (46).

The coefficients in the expression (33) for $\beta^{-1}(H)$ have the form

$$\alpha_1 = \sum_{nm} |\theta_n|^2 \exp(-4\pi i \rho n m - \pi \sigma (n^2 + 4m^2)),$$

$$\alpha_2 = \sum_{nm} |\theta_{n+1}|^2 \exp(-4\pi i \rho n m - \pi \sigma (n^2 + 4m^2)),$$

$$\alpha_3 = \sum_{nm} \theta_n \theta_{n+1} \exp(-2\pi i \rho n (2m+1) - \pi \sigma (n^2 + (2m+1)^2)),$$

$$Q_i = \sum_{nm} \theta_{n+i+1} \theta_{m+i+1} \theta_{n+m+i+1} (0,5 - \pi \sigma (n-m)^2) \times \exp(-2\pi i \rho n m - \pi \sigma (n^2 + m^2)),$$

$$\beta_0 = 2\sigma^{1/2} (|\theta_{\text{odd}}|^2 + |\theta_{\text{even}}|^2)^{-2} \sum_{nm} (\theta_{\text{even}}^* \theta_n \theta_m \theta_{n+m}^* + \theta_{n+1} \theta_{\text{odd}}^* \theta_{m+1} \theta_{n+m+1}^*) \times (1 + 2\gamma^2 (1 + 2b) (0,75 - \pi \sigma (n^2 + m^2) + \pi^2 \sigma^2 (m^2 - n^2)^2)) \times \exp(-2\pi i \rho n m - \pi \sigma (n^2 + m^2)).$$

The coefficients in (40) for a regular triangular TQL can be found numerically and equal

$$A_1 \approx 0,67 (1 + 2\gamma^2), \quad A_2 = \beta_0 \langle |\varphi_0|^2 \rangle^2 \approx 0,6 + 1,39\gamma^2 (1 + 2b),$$

$$B_1 \approx 0,53;$$

$$B_2 = \langle |G_F|^2 \rangle$$

$$= 0,25\sigma^{-1/2} \sum_{nm} (s_{\text{even}}^* s_n s_m s_{n+m}^* + s_{n+1} s_{\text{odd}}^* s_{m+1} s_{n+m+1}^*) \times \exp(-2\pi i \rho n m - \pi \sigma (n^2 + m^2)) \approx 0,38,$$

$$\langle |\varphi_0|^2 |G_F|^2 \rangle$$

$$= 0,25\sigma^{-1/2} \sum_{nm} (\theta_{\text{even}}^* \theta_n s_m s_{n+m}^* + \theta_{n+1} \theta_{\text{odd}}^* s_{m+1} s_{n+m+1}^*) \times \exp(-2\pi i \rho n m - \pi \sigma (n^2 + m^2)) \approx 0,24,$$

$$\langle |\varphi_2|^2 |G_F|^2 \rangle$$

$$= 0,25\sigma^{-1/2} \sum_{nm} (\theta_{\text{even}}^* \theta_n s_m s_{n+m}^* + \theta_{n+1} \theta_{\text{odd}}^* s_{m+1} s_{n+m+1}^*) \times (0,75 + \pi \sigma (-3n^2 + m^2) + \pi^2 \sigma^2 (m^2 - n^2)^2) \times \exp(-2\pi i \rho n m - \pi \sigma (n^2 + m^2)) \approx 0,95,$$

$$d_2 = \langle |\varphi_0|^2 \varphi_2^* G_F \rangle = -0,25 (s_{\text{odd}} Q_2^* + s_{\text{even}} Q_1^*) / \sigma^{1/2} \approx 0,31,$$

$$d_3 = 0,5 \langle \varphi_2^* G_F^2 \rangle = 0,125\sigma^{-1/2}$$

$$\times \sum_{nm} (\theta_n^* \theta_m^* s_{\text{even}} s_{n+m} + \theta_{n+1}^* \theta_{m+1}^* s_{\text{odd}} s_{n+m+1})$$

$$\times (0,75 - 3\pi \sigma (n-m)^2 + \pi^2 \sigma^2 (m-n)^4)$$

$$\times \exp(2\pi i \rho n m - \pi \sigma (n^2 + m^2)) \approx 0,$$

$$d_4 = \langle |G_F|^2 G_F \varphi_2^* \rangle = -0,25\sigma^{-1/2} (s_{\text{odd}} U_1^* + s_{\text{even}} U_0^*) \approx -0,24,$$

$$U_i = \sum_{nm} s_{n+i} \theta_{m+i} s_{n+m+i} (0,5 - \pi \sigma (n-m)^2) \times \exp(-2\pi i \rho n m - \pi \sigma (n^2 + m^2)).$$

Here θ_{even} and θ_{odd} are found from (10), if $x_0 = x'$, $y_0 = y'$, and s_{even} and s_{odd} from similar formulae for $x_0 = 5a_0/8$, $y_0 = -4b_0 \sin \alpha/3$.

The averaged quantities from (46) have the form (the case of a nonsingular single-quantum vortex lattice):

$$Z = \langle |\varphi_0|^2 |G|^2 \rangle = 0,5\sigma^{-1/2} \sum_{nm} \exp(2\pi i m (\tilde{x}_m/a_0 - n\rho) - \pi \sigma (m^2 + (n + \tilde{y}_m/(b_0 \sin \alpha))^2)),$$

$$\Gamma = 4 \langle |\varphi_2|^2 |G|^2 \rangle$$

$$= 2\sigma^{-1/2} \sum_{nm} (0,75 + \pi \sigma ((n + \tilde{y}_m/(b_0 \sin \alpha))^2 - 3m^2) + \pi^2 \sigma^2 ((n + \tilde{y}_m/(b_0 \sin \alpha))^2 - m^2)^2) \exp(2\pi i m (\tilde{x}_m/a_0 - n\rho) - \pi \sigma (m^2 + (n + \tilde{y}_m/(b_0 \sin \alpha))^2)),$$

$$\rho_2 = \sum_{nm} (0,5 - \pi \sigma (n - m + \tilde{y}_m/(b_0 \sin \alpha))^2) \times \exp(2\pi i m (\tilde{x}_m/a_0 - n\rho) - \pi \sigma (m^2 + (n + \tilde{y}_m/(b_0 \sin \alpha))^2)),$$

$$\times \exp(2\pi i m (\tilde{x}_m/a_0 - n\rho) - \pi \sigma (m^2 + (n + \tilde{y}_m/(b_0 \sin \alpha))^2)),$$

$$- \pi \sigma (m^2 + (n + \tilde{y}_m/(b_0 \sin \alpha))^2)),$$

$$\rho_1 = Q_1 (\theta_{\text{even}} = 1; \theta_{\text{odd}} = 1).$$

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Translated by E. Khmel'nitski