Structure of the vortex lattice in superconductors with a tricritical point

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Within the context of Ginzburg–Landau theory it is shown that in superconductors with a tricritical point near the second critical point the vortex lattice is energetically more favored, independent of the nature of the phase transition to the superconducting state in the absence of a magnetic field. © *1996 American Institute of Physics.* [S1063-7761(96)02001-9]

1. INTRODUCTION

With the discovery of new superconducting materials, interest has grown in the theoretical investigation of atypical superconductors. Earlier studies[1,2] have focused on the magnetic properties of superconductors with a tricritical point, i.e., those for which, depending on the thermodynamic parameters or composition of the material, the transition to the superconducting state can be either a first-order or second-order phase transition. Formally, this is expressed by a sign change in the coefficient of $|\psi|^4$ in the Ginzburg–Landau expansion of the free energy density, F_s in powers of the order parameter ψ, at some critical value of a controlling parameter, e.g., the pressure P:

$$F_s=F_n+a|\psi|^2+\frac{b}{2}|\psi|^4+\frac{d}{3}|\psi|^6. \tag{1}$$

Here F_n is the free energy density of the normal phase. The line $b(P,T)=0$ divides the PT plane into two regions: those of positive and negative values of b. In the region of positive b, the transition to the superconducting state takes place on the line $a(P,T)=0$ and is second-order. In the region of negative b, the transition takes place on the line $3b^2=16ad$ and is first-order. The two lines at the point where $a(P,T)=0$ and $b(P,T)=0$ simultaneously. This point is called the tricritical point. It is assumed that $d>0$ everywhere. In the BCS theory $b>0$; however, the next-order corrections to this theory in the small parameter T_c/ε_F frequently turn out to be larger than might have been expected from a simple estimate.[3]

It was shown in Refs. 1 and 2 that changing the sign of b, shows up in a striking way in the temperature–magnetic field phase diagram of the superconductor. It was also noted in these two references that the question of the symmetry of the vortex lattice for negative b requires additional study, since the usual arguments leading to stability of a triangular lattice[4,5] do not apply in this case. The goal of the present paper is the elucidate what sort of vortex lattice structure is most favorable for negative values of b. The existence of a stability region for a lattice other than triangular would mean that a phase transition at which the symmetry of the vortex lattice changes must take place in the vicinity of the tricritical point.

2. TRANSFORMATION OF THE FREE ENERGY

Near the tricritical point the fourth- and sixth-order terms in expansion (1) turn out to be equally important. This complicates the commonly used procedure[4] for finding the solution of the Ginzburg–Landau equations near H_{c2}. In this case it is more convenient to directly minimize the free energy. We will assume that the sample is a long cylinder with its axis parallel to the magnetic field **H**. It is necessary to minimize the free energy for a prescribed field

$$\tilde{\mathscr{F}}_s=\mathscr{F}_s-\int\frac{\mathbf{HB}}{4\pi}dV. \tag{2}$$

It is convenient to rewrite the expression for $\tilde{\mathscr{F}}_s$ in dimensionless form, using as the characteristic parameters the following quantities: the equilibrium value of the order parameter

$$\psi_0^2=(\sqrt{b^2-4ad}-b)/2d,$$

and the two characteristic lengths—the penetration depth λ and the correlation length ξ. They are expressed in terms of the coefficients a, b, and d as follows:

$$\lambda^2=mc^2/8\pi e^2\psi_0^2,\quad \xi^2=-\hbar^2/4m(2a+b\psi_0^2).$$

Hence, for the Ginzburg–Landau parameter we have

$$\kappa^2=\left(\frac{\lambda}{\xi}\right)^2=\frac{1}{2b_0}\sqrt{b^2-4ad},$$

where we have introduced the abbreviated notation $b_0=\pi(e\hbar/md)^2$. As a characteristic magnitude of the magnetic field we may use

$$H_0=\frac{\hbar c}{2e}\frac{1}{\xi\lambda}.$$

We now introduce the dimensionless quantities $\psi'=\psi/\psi_0$, $\mathbf{B}'=\mathbf{B}/H_0$, $\mathbf{A}'=\mathbf{A}/H_0\lambda$, and $F_s'=(8\pi/H_0^2)F_s$, where **B** is the magnetic induction and **A** is the corresponding vector potential, and we express all lengths in terms of λ. In the indicated units, we obtain the following expression for the difference of the free energies of the superfluid and normal phases $\Delta\tilde{\mathscr{F}}$:

$$\Delta\tilde{\mathcal{F}}=\int\left[(\mathbf{B}-\mathbf{H}_e)^2+\left|\left(-i\frac{\nabla}{\kappa}-\mathbf{A}\right)\psi\right|^2-\frac{1+\theta}{2}|\psi|^2\right.$$
$$\left.+\frac{\theta}{2}|\psi|^4+\frac{1-\theta}{6}|\psi|^6\right]dV, \tag{3}$$

where $\mathbf{H}_e$ is the external magnetic field. One more dimensionless parameter besides the Ginzburg–Landau parameter enters into the above expressi

$$\theta=b/\sqrt{b^2-4ad}.$$

This parameter derives from the extra coefficient d in the initial expression for the free energy density (1).

For a given external field $\mathbf{H}_e$ the order parameter ψ and the magnetic induction $\mathbf{B}$ can be found by minimizing $\Delta\tilde{\mathcal{F}}$. We perform this minimization via successive approximation in the small parameters $H_{c2}-H_e$ and $|\psi|^2$. Varying $\Delta\tilde{\mathcal{F}}$ with respect to $\mathbf{B}$ in the zeroth approximation in the indicated parameters gives

$$\mathbf{B}=\mathbf{H}_e. \tag{4}$$

In the next approximation, dropping terms in the functional (3) of order $|\psi|^4$ and $|\psi|^6$ and varying the remaining expression with respect to ψ^*, we obtain the linear equation

$$\left(-i\frac{\nabla}{\kappa}-\mathbf{A}\right)^2\psi-\frac{1+\theta}{2}\psi=0. \tag{5}$$

In this equation $\mathrm{curl}\mathbf{A}=\mathbf{B}=\mathbf{H}_e$ by virtue of (4). Proceeding in the usual way,[4] we find the upper critical field

$$H_{c2}=\kappa(1+\theta)/2$$

as the field at which a bounded solution first appears:

$$\psi\sim\exp\left\{ikx-\frac{\kappa H_{c2}}{2}\left(y-\frac{k}{\kappa H_{c2}}\right)^2\right\}. \tag{6}$$

This solution is degenerate in the position of the center of the orbit $k/\kappa H_{c2}$. The periodic solution describing the entire structure of the superconducting vortices near H_{c2} is sought in the form of a linear combination of functions of the form (6):

$$\Psi=\sum_{n=-\infty}^{\infty}C_n\exp\left\{iknx-\frac{\kappa B}{2}\left(y-\frac{kn}{\kappa B}\right)^2\right\}. \tag{7}$$

Substituting the functions (7) into Eq. (3) gives

$$\Delta\tilde{\mathcal{F}}=\int\left[(B-H_e)^2+\left(\frac{B}{\kappa}-\frac{1+\theta}{2}\right)|\psi|^2+\frac{\theta}{2}|\psi|^4\right.$$
$$\left.+\frac{1-\theta}{6}|\psi|^6\right]dV, \tag{8}$$

Here, as in Eq. (7), the field B is assumed to be homogeneous. Varying the above expression with respect to B gives the first-order correction in $|\psi|^2$ to relation (4):

$$B=H_e-\frac{\langle|\psi|^2\rangle}{2\kappa}, \tag{9}$$

where

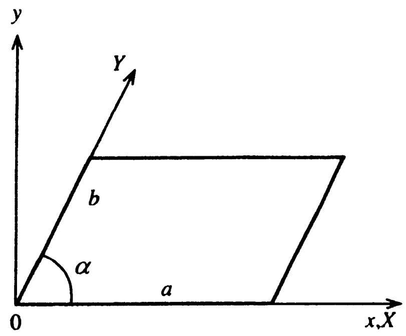

FIG. 1. Unit cell.

$$\langle|\psi|^2\rangle=\frac{1}{V}\int|\psi|^2dV.$$

Substituting Eq. (9) into Eq. (8) allows us to express $\Delta\tilde{\mathcal{F}}$ in terms of the means of the powers of the order parameter:

$$\Delta\tilde{\mathcal{F}}=\frac{H_e-H_{c2}}{\kappa}\langle|\psi|^2\rangle+\frac{1}{2}\left(\theta-\frac{1}{2\kappa^2}\right)\langle|\psi|^4\rangle$$
$$+\frac{1-\theta}{6}\langle|\psi|^6\rangle. \tag{10}$$

We now have in mind substituting the order parameter ψ in the form (7). The coefficients C_n are related in a way that depends on the exact form of the periodic structure under consideration. The unit cell in general is a parallelogram with sides a and b and acute angle α (see Fig. 1). One quantum of magnetic flux should be assigned to the unit cell. This imposes a constraint on the lattice parameters:

$$abH_{c2}|\sin\alpha|=\frac{2\pi}{\kappa}. \tag{11}$$

After allowing for this constraint in the solution (7), the degeneracy with respect to the three continuous parameters remains. This can be the ratio of the main periods of the structure $R=b/a$, the angle α between the basis vectors, and the total amplitude of the solution, e.g., $\langle|\psi|^2\rangle$. To remove this degeneracy, we must minimize expression (10) and find "the correct zeroth-approximation functions." In this way the coefficients C_n and the lattice parameters are determined.

The minimization with respect to $\langle|\psi|^2\rangle$ can be completed by introducing the ratios

$$\beta=\frac{\langle|\psi|^4\rangle}{\langle|\psi|^2\rangle^2},\quad \gamma=\frac{\langle|\psi|^6\rangle}{\langle|\psi|^2\rangle^3}. \tag{12}$$

These ratios depend only on the lattice parameters. The expression for $\Delta\tilde{\mathcal{F}}$ in terms of β and γ

$$\Delta\tilde{\mathcal{F}}=\frac{H_e-H_{c2}}{\kappa}\langle|\psi|^2\rangle+\frac{1}{2}\left(\theta-\frac{1}{2\kappa^2}\right)\beta\langle|\psi|^2\rangle^2$$
$$+\frac{1-\theta}{6}\gamma\langle|\psi|^2\rangle^3 \tag{13}$$

is analogous to its initial form (1), except that the role of the order parameter is now played by $\langle|\psi|^2\rangle$, and the controlling parameter instead of the temperature is H_e-H_{c2}.

For subsequent minimization of the free energy it is convenient to introduce the following abbreviated notation:

$$\epsilon=\frac{H_e-H_{c2}}{\kappa},\quad \mu=\beta\left(\theta-\frac{1}{2\kappa^2}\right),\quad \nu=\frac{1-\theta}{2}\gamma.$$

After minimizing with respect to $\langle|\psi|^2\rangle$, we obtain the following expression for the difference of the free energies of the superconducting and normal phases:

$$\Delta\tilde{\mathcal{F}}=-\frac{1}{24\nu^2}(\sqrt{\mu^2-4\epsilon\nu}-\mu)^2(2\sqrt{\mu^2-4\epsilon\nu}+\mu). \tag{14}$$

The phase transition takes place when $\Delta\tilde{\mathcal{F}}=0$. For $\mu>0$ the first expression in parentheses may vanish, which would correspond to a second-order transition for $\varepsilon=0$, i.e., $H=H_{c2}$. For $\mu<0$ the second expression in parentheses vanishes, which corresponds to a first-order transition on the line defined by the equation

$$\varepsilon=3\mu^2/16\nu, \tag{15}$$

i.e., for $H>H_{c2}$.

3. GEOMETRY OF THE VORTEX LATTICE

Following Ref. 5, we seek a periodic solution (vortex lattice) with unit cell in the form of a parallelogram (Fig. 1). In the coordinates X,Y, for which

$$x=X+Y\cos\alpha,\quad y=Y\sin\alpha,$$

the solution takes the form

$$|\Psi(X,Y)|=|C_0|\left|\sum_{n=-\infty}^{\infty}\exp\left(i\pi n(n-1)\frac{b}{a}\cos\alpha\right)\times\exp\left(\frac{2i\pi n}{a}(X+Y\cos\alpha)\right)\right|\times\left|\exp\left(-\frac{\kappa H_{c2}}{2}(Y+bn)^2\sin^2\alpha\right)\right|. \tag{16}$$

After substituting this expression into definitions (12) and then, allowing for relation (11), into formula (14) for the free energy, the free energy becomes a function of the two variables $R=b/a$ and α, which can be combined into one complex variable

$$z=Re^{i\alpha}=u+iv,$$

and the problem of finding the most favored lattice structure reduces to minimizing a function of two variables

$$F(u,v)=\Delta\mathcal{F}(\mu(u,v),\nu(u,v)).$$

The condition for an extremum of this function in u and v takes the form

$$\Delta\tilde{\mathcal{F}}_\mu\mu_u+\Delta\tilde{\mathcal{F}}_\nu\nu_u=0,\quad \Delta\tilde{\mathcal{F}}_\mu\mu_v+\Delta\tilde{\mathcal{F}}_\nu\nu_v=0, \tag{17}$$

where $\Delta\tilde{\mathcal{F}}_\mu=\partial\Delta\tilde{\mathcal{F}}/\partial\mu$, etc.

These conditions are satisfied in two cases: 1) $\mu_u\nu_v-\nu_u\mu_v\neq 0$, whereupon we have $\Delta\tilde{\mathcal{F}}_\mu=\Delta\tilde{\mathcal{F}}_\nu=0$, or 2) $\mu_u\nu_v-\nu_u\mu_v=0$.

By direct differentiation of expression (14) we obtain

$$\Delta\tilde{\mathcal{F}}_\mu=\frac{1}{8\nu^2}(\sqrt{\mu^2-4\nu\varepsilon}-\mu)^2,$$

$$\Delta\tilde{\mathcal{F}}_\nu=\frac{1}{12\nu^3}(\sqrt{\mu^2-4\nu\varepsilon}-\mu)\times(\mu^2-2\nu\varepsilon-\mu\sqrt{\mu^2-4\nu\varepsilon}).$$

Case 1) coincides with the condition for the vanishing of the function F itself and defines the line of second-order phase transitions $\varepsilon=0$, $\mu>0$.

Case 2) reduces to a condition for β and γ:

$$\beta_u\gamma_v-\beta_v\gamma_u=0. \tag{18}$$

This condition is obviously fulfilled if $\beta_u=\beta_v=\gamma_u=\gamma_v=0$, i.e., at the global extrema of β and γ. In this case, no constraints are imposed on $\Delta\tilde{\mathcal{F}}_\mu$ and $\Delta\tilde{\mathcal{F}}_\nu$.

If any of the derivatives of the functions β and γ are equal to zero, then $\Delta\tilde{\mathcal{F}}_\mu$ and $\Delta\tilde{\mathcal{F}}_\nu$ are connected by one relation, for which we may take, for example, the second of conditions (17). This relation can be reduced to the form

$$3\frac{\beta_v}{\gamma_v}\left(\beta-\frac{3}{2}\gamma\frac{\beta_v}{\gamma_v}\right)=\frac{\varepsilon(1-\theta)}{(\theta-1/2\kappa^2)^2}. \tag{19}$$

For further analysis, it is necessary to know the properties of the functions β and γ.

The function $\beta(R,\alpha)$ has been investigated in Ref. 5, where it was determined that

$$\beta=\sqrt{v}\left(\left|\sum_{n=-\infty}^{\infty}\exp(2\pi in^2z)\right|^2+\left|\sum_{n=-\infty}^{\infty}\exp\left[2\pi i\left(n+\frac{1}{2}\right)^2z\right]\right|^2\right). \tag{20}$$

It was also shown there that $\beta(u,v)$ possesses the following symmetry properties:

1) β is periodic in u with period 1: $\beta(u+1)=\beta(u)$;

2) β is symmetric with respect to the $u=1/2$ axis: $\beta(1-u)=\beta(u)$;

3) β is symmetric with respect to inversion about the unit circle centered at $z=0$: $\beta(1/z^*)=\beta(z)$.

These properties express the invariance of the function β with respect to the choice of the unit cell of the lattice.

The properties of the function $\gamma(z)$ are considered in the Appendix, where it is shown that $\gamma(z)$ reduces to the form

$$\gamma=\frac{2}{\sqrt{3}}v(|f_0g_0+f_1g_3|^2+2|f_0g_2+f_1g_1|^2), \tag{21}$$

where

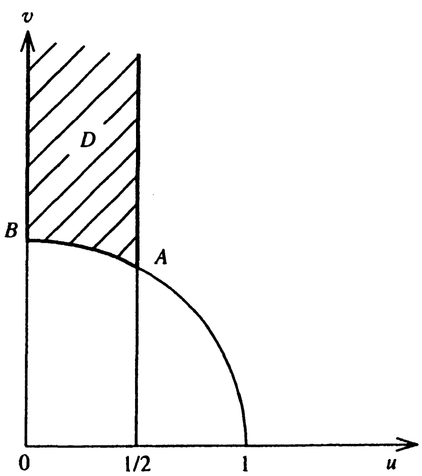

FIG. 2. The region D.

$$f_t = \sum_{q=-\infty}^{\infty} \exp\left[\frac{\pi}{2} iz(2q+t)^2\right],$$

$$g_p = \sum_{r=-\infty}^{\infty} \exp\left[\frac{\pi}{6} iz(6r+p)^2\right].$$

By virtue of the requirement of invariance with respect to the choice of basis, the function $\gamma(z)$ possesses the same symmetry properties as $\beta(z)$, i.e.,

1) $\gamma(u+1)=\gamma(u)$,

2) $\gamma(1-u)=\gamma(u)$,

3) $\gamma(1/z^*)=\gamma(z)$.

These properties can be checked by reference to the representation of $\gamma(z)$ given by Eq. (21). Thanks to the enumerated symmetry properties, it is sufficient to consider $\beta(z)$ and $\gamma(z)$ only in the region D of the uv plane (the hatched region) in Fig. 2. As in the case of ordinary superconductors,[5] it follows from symmetry properties 1 and 2 that $\beta_u=0$ and $\gamma_u=0$ on the lines $u=0$ and $u=1/2$, and thus Eq. (18) is satisfied on the indicated lines. By virtue of property 3 this equation is also satisfied on the arc $z=\exp(i\alpha)$, $\pi/3<\alpha<\pi/2$, i.e., condition (18) is satisfied everywhere on the boundary of the region D.

Numerical analysis of Eq. (18) shows that inside the region D it has no solutions. Thus, the conditions of an extremum (17) can be fulfilled only on the boundary of the region D. At the intersection points of the lines bounding the region D (the points A and B in Fig. 2), by virtue of properties 1–3, the derivatives of $\beta(z)$ and $\gamma(z)$ should vanish in both directions: $\beta_u=\beta_v=0$ and $\gamma_u=\gamma_v=0$, i.e., at these points both $\beta(z)$ and $\gamma(z)$ have extrema.

An important, general property of the functions β and γ is that for any given $u \in D$ they grow monotonically with v, and for any given $v \in D$ they grow monotonically with u. This property can be established for large v analytically, and for any finite v—numerically. It follows from this property that the point A is a minimum of β and γ, and the point B—a saddle point. A surface plot of $\gamma(z)$ is shown in Fig. 3.

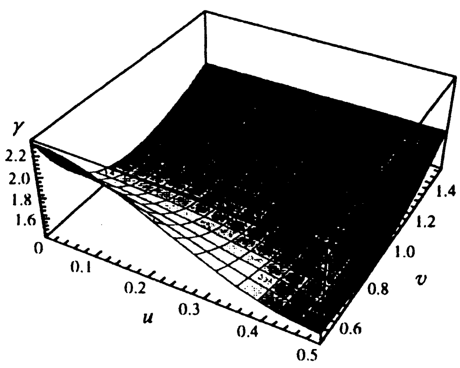

FIG. 3. Surface plot of the function $\gamma(z)$, $z=u+iv$.

By virtue of (17), $F(u,v)$ will also have an extremum at A and B for any values of the parameters κ, θ, and ε. Point A corresponds to a triangular lattice, and point B—to a square lattice. In the case of an ordinary superconductor, $\Delta\mathcal{F}$ reaches its minimum where β has its minimum. Therefore, in the ordinary case the triangular lattice is the equilibrium lattice.[5,6] In the case considered here, β and γ enter into the expression for $\Delta\tilde{\mathcal{F}}$ with coefficients which can have different signs. For this reason, a global minimum of β or γ does not have to be a minimum of $\Delta\tilde{\mathcal{F}}$.

In addition, $\Delta\tilde{\mathcal{F}}$ can have extrema on the boundary of the region D. In order to find these extrema, we rewrite condition (19) in the form

$$\varepsilon = G(u,v)\varepsilon_0,$$

where we have introduced the notation

$$G(u,v) = 8\left(\beta - \frac{3}{2}\gamma\frac{\beta_v}{\gamma_v}\right)\frac{\beta_v}{\gamma_v}, \tag{22}$$

$$\varepsilon_0(\kappa,\theta) = \frac{3(\theta - 1/2\kappa^2)^2}{8(1-\theta)}. \tag{23}$$

Condition (19) should be considered only on the boundary of the region D. Numerical analysis shows that on this boundary the function $G(u,v)$ varies in the following way:

1) on the lines $u=0$ and $u=1/2$ it decays monotonically with v and tends toward the limit $G(u,\infty)=G_\infty=\sqrt{3}/2$;

2) on the line $R=1$, $\pi/3<\alpha<\pi/2$ it decays monotonically together with α;

3) $G(A)=G_A=1.2557$.

Since $G(u,v)$ varies within finite limits, additional extrema exist only for $G_\infty<\varepsilon/\varepsilon_0<G_A$. A study of the second derivatives shows that for $\varepsilon/\varepsilon_0=G_A$ the nature of the extremum of F changes at the point A. For $\varepsilon/\varepsilon_0>G_A$ this extremum is a maximum, and for $\varepsilon/\varepsilon_0<G_A$ it is a minimum. Thus, the line $\varepsilon=\varepsilon_0 G_A$ is the boundary of stability of the triangular lattice. In the interval $1<\varepsilon/\varepsilon_0<G_A$ the triangular lattice, and with it the superconducting phase, exist as a metastable state ($\Delta\tilde{\mathcal{F}}>0$). The value $\varepsilon=\varepsilon_0$ corresponds to a first-order transition to the mixed state (see formula (15)). For $\varepsilon=\varepsilon_0 G_A$, simultaneous with the change in the nature of the extremum at the point A two additional extrema of F arise, one on the line $u=1/2$, and the other on the arc

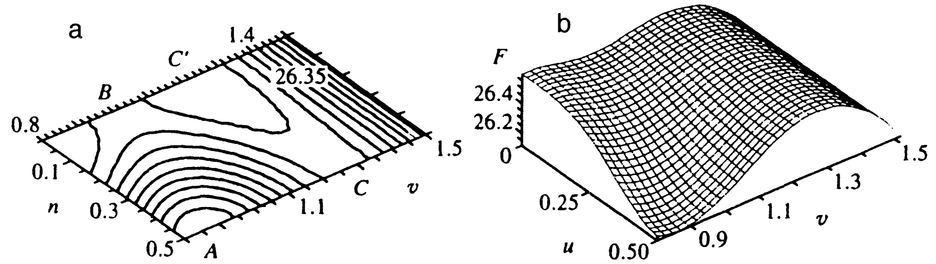

FIG. 4. Contour plot (a) and surface plot (b) of $F(u,v)$ for $G_\infty<\varepsilon/\varepsilon_0<G_B$. The positions of the extrema are indicated on the contour plot: A ($z=\exp(i\pi/3)$) is a minimum, B ($z=i$) is a saddle point, and C and C' are additional extrema.

$R=1$, $\pi/3<\alpha<\pi/2$. With further decrease of ε these extrema move away from the point A along the segments of the boundary of the region D intersecting at A. Neither of the additional extrema is a minimum; however, as they move, the nature of the extremum at B can change. For $\varepsilon/\varepsilon_0=1.2376$, when one of the extrema falls on the point B, the saddle point at this point becomes a maximum, and for $\varepsilon/\varepsilon_0=G_B=1.2142$ it becomes once again a saddle point. As $\varepsilon/\varepsilon_0\to G_\infty$ both additional extrema move out to infinity along the lines $u=0$ and $u=1/2$. For $\varepsilon/\varepsilon_0<G_\infty$ the function F has only two extrema—a minimum at A and a saddle point at B.

Thus, over the entire existence region of the superconducting phase the point A, corresponding to a triangular lattice, is the only minimum of $\Delta\tilde{\mathcal{F}}$. No other lattices, include a square lattice, can exist, even as metastable states. The point B, corresponding to a square lattice, is not a minimum for any ε.

4. CONCLUSION

The above analysis shows that in superconductors with a tricritical point a triangular vortex lattice is stable over the entire existence region of the superconducting phase. For this reason, phase transitions associated with a change in the structure of the vortex lattice should not take place. The triangular lattice is stable also in the region where the superconducting phase is metastable, i.e., for

$$1<\frac{8}{3}\frac{1-\theta}{(\theta-1/2\kappa^2)^2}\frac{H-H_{c2}}{\kappa}<1.2557. \tag{24}$$

The existence of hysteresis at the transition to the mixed state and the existence of a region of metastability can be used experimentally to search for superconductors with a tricritical point.

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APPENDIX A CALCULATION OF $\gamma(z)$

In the dimensionless variables $\xi=Y/b$ and $\eta=X/b$ formula (16) for $|\Psi|$ takes the form

$$|\Psi(\xi,\eta)|=|C_0|\left|\sum_{n=-\infty}^{\infty}\exp[i\pi n(n-1)R\cos\alpha]\times\exp[2i\pi nR(\eta+\xi\cos\alpha)]\right|\times|\exp[-\pi R(\xi+n)^2|\sin\alpha|]|, \tag{A1}$$

where $R=b/a$.

This function is periodic in ξ with period 1 and in η with period $a/b=1/R$.

Then for $|\Psi|^6$ we obtain

$$|\Psi|^6=|C_0|^6\sum_{n,k=-\infty}^{\infty}\exp\{i\pi[n_1(n_1-1)+n_2(n_2-1)+n_3(n_3-1)+k_1(k_1-1)+k_2(k_2-1)+k_3(k_3-1)]R\cos\alpha\}\exp[2i\pi(n_1+n_2+n_3-k_1-k_2-k_3)R(\eta+\xi\cos\alpha)]\exp\{-\pi R[(\xi-n_1)^2+(\xi-n_2)^2+(\xi-n_3)^2+(\xi-k_1)^2+(\xi-k_2)^2+(\xi-k_3)^2]|\sin\alpha|\}. \tag{A2}$$

Averaging over η, we have

$$\langle|\Psi|^6\rangle_\eta=|C_0|^6\sum_{n,k=-\infty}^{\infty}\exp\{i\pi[n_1(n_1-1)+n_2(n_2-1)+n_3(n_3-1)+k_1(k_1-1)+k_2(k_2-1)+k_3(k_3-1)]R\cos\alpha\}\exp\{-\pi R[(\xi-n_1)^2+(\xi-n_2)^2+(\xi-n_3)^2+(\xi-k_1)^2+(\xi-k_2)^2+(\xi-k_3)^2]|\sin\alpha|\}, \tag{A3}$$

where the sum is taken over the points in the P plane:

$$n_1+n_2+n_3=k_1+k_2+k_3. \tag{A4}$$

Denoting k_i as n_{i+3} for $i=1,2,3$ and taking Eq. (A4) into account, we transform the argument of the second exponential:

$$\sum_{i=1}^{6}(\xi-n_i)^2=6\left(\xi+\frac{1}{6}\sum_{i=1}^{6}n_i\right)^2+\frac{1}{6}\left(6\sum_{i=1}^{6}n_i^2-\left(2\sum_{i=1}^{3}n_i\right)^2\right)=6\left(\xi+\frac{1}{6}\sum_{i=1}^{6}n_i\right)^2$$

$$+\frac{1}{3}[(n_1-n_2)^2+(n_2-n_3)^2+(n_1-n_3)^2+(k_1-k_2)^2+(k_2-k_3)^2+(k_1-k_3)^2]. \quad \text{(A5)}$$

We make a change of variables (the summation indices) that diagonalizes the quadratic form inside the brackets and transforms the form inside the parentheses into a new variable:

$$N=n_1+n_2+n_3=k_1+k_2+k_3,\quad q_n=n_1-n_2,$$
$$r_n=3n_3-N=2n_3-n_1-n_2, q_k=k_1-k_2, \quad \text{(A6)}$$
$$r_k=3k_3-N=2k_3-k_1-k_2.$$

For the new indices N, q_n, r_n, q_k, and r_k, the summation condition (A3) is fulfilled automatically.

The back substitution for the n_i has the form

$$6n_1=2N-r_n+3q_n,\quad 6n_2=2N-r_n-3q_n,$$
$$3n_3=N+r_n. \quad \text{(A7)}$$

Thus

1) $(n_1-n_2)^2+(n_2-n_3)^2+(n_3-n_1)^2=(3q_n+r_n)/2$,

2) $n_1(n_1-1)+n_2(n_2-1)+n_3(n_3-1)=n_1^2+n_2^2+n_3^2-N$
$=N^2-N-2(n_1n_2+n_1n_3+n_2n_3)$,

3) $n_1n_2+n_1n_3+n_2n_3=(4N-r_n-3q_n)/12$

and analogously for k_i. The expression in brackets in the first exponential takes the form

$$n_1(n_1-1)+n_2(n_2-1)+n_3(n_3-1)-k_1(k_1-1)-k_2(k_2-1)-k_3(k_3-1)=(r_n^2+3q_n^2-r_k^2-3q_k^2)/12,$$

and Eq. (A3) becomes

$$\langle|\Psi|^6\rangle_\eta=|C_0|^6\sum_{[r,q,N]}^{\infty}\exp\left[\frac{i\pi R\cos\alpha}{6}(r_n^2+3q_n^2-r_k^2-3q_k^2)\right]\exp\left[6\pi R\sin\alpha\left(\xi-\frac{N}{3}\right)^2\right]\exp\left[\frac{-\pi R\sin\alpha}{6}(3q_n^2+r_n^2+3q_k^2+r_k^2)\right]$$
$$=|C_0|^6\sum_{[r,q,N]}^{\infty}\exp\left[-6\pi v\left(\xi-\frac{N}{3}\right)^2\right]\exp\left\{\frac{\pi}{6}[iz(3q_n^2+r_n^2)+(iz)^*(3q_k^2+r_k^2)]\right\}, \quad \text{(A8)}$$

where $z=Re^{i\alpha}=u+iv$.

The summation over the indices r, q, and N in expression (A8) is subject to restrictions stemming from out of relations (A6), which are indicated symbolically by the bracketed expression under the summation sign. The numbers N define planes cutting off equal segments along the n_1, n_2, and n_3 axes. The location of integer sites on neighboring planes is not identical. It repeats every three planes. Therefore we must introduce an additional index p distinguishing planes of different type, i.e., we must set

$$N=3N'-p,\ \text{where } N' \text{ is an integer},\quad p=1,2,3 \times(\text{or} -1,0,1;\ \ldots). \quad \text{(A9)}$$

From the definition of r_n and r_k it is obvious that these numbers should have the form

$$r_n=3r_n'+p,\quad r_k=3r_k'+p, \quad \text{(A10)}$$

where r_n' and r_k' are integer, and $p=1,2,3$ (or $-1,0,1$; ...).

We then obtain from Eq. (A8)

$$\langle|\Psi|^6\rangle_\eta=|C_0|^6\sum_{p=1}^{3}\sum_{N'=-\infty}^{\infty}\exp\left[-6\pi v\left(\xi-\frac{3N'-p}{3}\right)^2\right]\times\sum_{[r_n',q_n]}^{\infty}\exp\left\{\frac{\pi}{6}iz[3q_n^2+(3r_n'+p)^2]\right\}\times\sum_{[r_k',q_k]}^{\infty}\exp\left\{\frac{\pi}{6}(iz)^*[3q_k^2+(3r_k'+p)^2]\right\}. \quad \text{(A11)}$$

After averaging over ξ we have

$$\langle|\Psi|^6\rangle=|C_0|^6\langle\ldots\rangle_\xi\sum_{p=1}^{3}\left|\sum_{[r',q]}^{\infty}\exp\left\{\frac{\pi}{6}iz[3q^2+(3r'+p)^2]\right\}\right|^2, \quad \text{(A12)}$$

where

$$\langle\ldots\rangle_\xi=\left\langle\sum_{N'=-\infty}^{\infty}\exp\left[-6\pi v\left(\xi-\frac{3N'-p}{3}\right)^2\right]\right\rangle_\xi=\int_0^1\sum_{N'=-\infty}^{\infty}\exp\left[-6\pi v\left(\xi-N'+\frac{p}{3}\right)^2\right]d\xi=\frac{1}{\sqrt{6v}},$$

Yet another restriction is associated with the fact that for even N the numbers n_3 and n_1+n_2, and therefore n_1-n_2, must have identical parity, and for odd N, different. In order to allow for this, we must introduce another parameter t which takes two values (0 and 1) according to the rule

$$r'=2r''+t \quad \text{and} \quad q=2q'+t+p,$$

where r'' and q' are integers, $t=0,1$, and $p=0,1,2$.

With there definitions, the formulas linking the old indices n_1, n_2, and n_3 with the new ones N', r', and q' are

$$2n_1==2N'-r'+q-p,\quad 2n_2=2N'-r'-q-p, \quad \text{(A13)}$$
$$n_3=N'+r'.$$

The expression inside the absolute value sign in Eq. (A12) after this substitution takes the form

$$\sum_{t=0}^{1}\sum_{q'=-\infty}^{\infty}\exp\left[\frac{\pi}{2}iz(2q'+t)^2\right]\sum_{r''=-\infty}^{\infty}$$
$$\times\exp\left[\frac{\pi}{6}iz(6r''+2p+3t)^2\right]. \tag{A14}$$

We introduce the notation

$$f_t=\sum_{q=-\infty}^{\infty}\exp\left[\frac{\pi}{2}iz(2q+t)^2\right], \tag{A15}$$

$$g_p=\sum_{r=-\infty}^{\infty}\exp\left[\frac{\pi}{6}iz(6r+p)^2\right]. \tag{A16}$$

Then expression (A14) reduces to

$$\sum_{p=0}^{2}\left|\sum_{t=0}^{1}f_t g_{3t+2p}\right|^2=|f_0g_0+f_1g_3|^2+2|f_0g_2+f_1g_1|^2. \tag{A17}$$

Noting that $\langle|\Psi|^2\rangle=|C_0|^2/\sqrt{2v}$, we finally obtain

$$\gamma=\frac{2}{\sqrt{3}}v(|f_0g_0+f_1g_3|^2+2|f_0g_2+f_1g_1|^2). \tag{A18}$$

Symmetry properties 1 and 2 are established by a direct check. To prove property 3, we express all of the functions on the right-hand side of Eq. (A18) in terms of f_0:

$$f_1(z)=f_0(z/4)-f_0(z),\quad g_0(z)=f_0(3z),$$

$$g_1(z)=\frac{1}{2}\left[f_0\left(\frac{z}{12}\right)+f_0(3z)-f_0\left(\frac{z}{3}\right)-f_0\left(\frac{3z}{4}\right)\right],$$

$$g_2(z)=\frac{1}{2}\left[f_0\left(\frac{z}{3}-f_0(3z)\right)\right],$$

$$g_3(z)=f_0(3z/4)-f_0(3z).$$

It is then necessary to apply the Poisson sum formula

$$\sum_{k=-\infty}^{\infty}f(k)=\sum_{k=-\infty}^{\infty}\int_{-\infty}^{\infty}f(x)e^{2\pi ikx}dx. \tag{A19}$$

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