Influence of quenched disorder on the square-to-rhombohedral structural transformation of the vortex lattice of type-II superconductors

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A theory of structural transformations of the vortex lattice in a disordered fourfold symmetric type-II superconductor is constructed using two complementary descriptions of the vortex matter. At low temperatures we use a nonlocal London approach, while near $H_{c2}(T)$ the lowest Landau level Ginzburg-Landau model with an asymmetric high derivative term is utilized. The quenched disorder influences the location of the square-to-rhombohedral structural transition line, the simplest transformation of that kind. In the clean case the slope of the line in the *T*-*B* plane is generally negative, as thermal fluctuations favor a more symmetric square lattice. We calculated the transition line in the presence of pinning and find that the disorder, which plays an important role in low-T_c materials, makes the slope positive, as has been observed in recent experiments.

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I. INTRODUCTION

Structural phase transitions (SPTs) in crystalline systems are an old and still not sufficiently well developed branch of the physics of phase transitions, partly because of the difficulty in controlling such a transition in atomic crystals. However, structural phase transitions are not restricted to atomic crystals. In particular, vortices in superconductors in the presence of a magnetic field repel each other and also arrange themselves in various two-dimensional lattice structures. Transformation between these structures offer a convenient experimental system in which to investigate such a transition (in a simplified two-dimensional form), since it can be effectively triggered by modifying both the magnetic field, which determines the density of vortices, and the temperature. The improved quality of single crystals of various new anisotropic superconductors, like the high-T_c cuprates or relatively low-T_c materials, recently allowed clear identification of the structural phase transitions between various vortex lattice states by means of small-angle neutron scattering, scanning tunneling spectroscopy, and decoration experiments. The simplest transition of that kind is the square-to-rhombohedral transformation in the vortex lattice in fourfold symmetric systems. In a typical case, a single crystal of the tetragonal material (like those of the borocarbide family) are placed in an external magnetic field oriented along the crystallographic *c* axis to preserve the fourfold symmetry in the basal *a*-*b* plane. The clearest observations of this SPT are obtained in borocarbide materials $LuNi_2B_2C$,[1–4] and YNi_2B_2C,[5] which have nonmagnetic rare-earth ions and do not introduce any complications to the mixed state due to competition between magnetism and superconductivity.

The precise location in the *T*-*H* plane of the critical line of the square-rhombohedral SPT in the vortex crystal is still a matter of discussion. Earlier experiments on $LuNi_2B_2C$ indicate a very small positive slope of the transition line in the *T*-*B* plane $H_2(T)$ till it reaches the $H_{c2}(T)$ region. Then, according to some experiments,[2,3] it abruptly turns up and even acquires a negative slope at high fields, while in other experiments in a closely related material YNi_2B_2C,[5] it continues the gradual increase even near $H_2(T)$. The results at low temperatures was first explained in the framework of the nonlocal London (NLL) theory proposed by Kogan and collaborators.[6] The NLL theory includes four derivative terms which bring in the anisotropy effects essential to trigger the SPT between the vortex lattice phases. The more symmetric square vortex crystal, stable at a stronger magnetic field (higher density of vortices), transforms into a less symmetric rhombic vortex crystal as the magnetic field decreases. Thus the square-to-rhombohedral SPT is associated with a spontaneous breaking of the fourfold symmetry of the system. The transition has also been understood theoretically on the basis of the Ginzburg-Landau functional which had to be extended in a similar fashion, by including an asymmetric four derivative term.[7] Such higher derivatives Ginzburg-Landau (HDGL) theories are applicable, strictly speaking, not far from T_c, but they generally work well in a much larger part of the *T*-*H* plane, including fields and temperatures well below the $H_{c2}(T)$ line.[8]

Although temperature might be introduced into these phenomenological models via a temperature dependence of their coefficients, the resulting slope of the transition line is typically very small and, more importantly, is of higher order in the relevant expansion parameter and therefore cannot be predicted. It should be emphasized at this point that both NLL and HDGL were solved at the mean-field level only in the papers mentioned above and only recently in Refs. 9 and 10, respectively, were attempts made to take into account thermal fluctuations on the "mesoscopic" scale. Although thermal fluctuations are dominant in high-T_c superconductors, leading, for example, to the vortex lattice melting,[11] they are negligible in low-T_c materials for which the Ginzburg number, characterizing the strength of the thermal fluctuations, is several orders of magnitude lower. In high-T_c superconductors the square-to-rhombohedral transition was observed directly via neutron scattering in $YBa_2Cu_3O_{7+\delta}$,[12] and $La_2Sn_{1-x}Cu_xO_4$ (LaSCO),[13] and indirectly via the peak effect[14] in LaSCO. At least in LaSCO the transition line exhibits negative slope in the T-H plane (at odds with theory[9,10]). In the previous paper[15] we calculated the effect of significant thermal fluctuations on the transition using the self-consistent harmonic approximation within NLL and found a negative slope. This conclusion is supported by an argument that the more symmetric phase generally appears at higher temperatures.

In all the theoretical papers mentioned above disorder was neglected. The general argument about the slope of the transition line, however, breaks down when quenched disorder is involved. While thermal fluctuations generally expand the available phase space, quenched disorder tends to do the opposite: the phase space shrinks. This conclusion is of a very general nature. It applies, for example, to the vortex lattice melting. The liquid phase is the symmetric one, while the crystalline phase breaks the rotation and translation symmetries. Indeed when the thermal fluctuations dominate (above the Kauzmann point) the melting line exhibits a negative slope, while when the disorder dominates the slope become positive (this feature was termed "inverse melting"[13,14,16]). In low-T_c superconductors disorder is more important than thermal fluctuations (which are negligible in most cases) and this motivates us to consider the disorder using both the GL theory with asymmetric four derivative terms included and NLL. Our conclusion is that, as generally expected, the critical line bends up in both cases, enlarging the domain in the parameter space occupying by the less symmetric phase.

The rest of the paper is organized as follows. We start in Sec. II with the anisotropic London model to which quenched disorder is added. In Sec. III the theory of the transition within the anisotropic Ginzburg-Landau model is presented, followed by a discussion and conclusions in Sec. IV.

II. LONDON APPROACH

We use here an extension of the standard London theory of vortex matter to include an anisotropic part of the interaction between flux lines already used in Ref. 15. Since thermal fluctuations on the mesoscopic scale are small we neglect them here and discuss them later.

A. Disordered NLL model

For a strongly type-II superconductor ($\kappa \equiv \lambda/\xi \gg 1$), isotropic in the a-b plane, the potential of the interaction between two parallel straight vortex lines at zero temperature is known to be well approximated by[17]

$$V(r) = \frac{\Phi_0^2}{8\pi^2\lambda^2}[K_0(r/\lambda) - K_0(r/\xi)], \tag{1}$$

where r is the distance between the vortices. The repulsive part of this potential is due to the long-range magnetic interactions, while the attractive part is due to the overlap of the vortex cores. Note that despite the fact that both terms in Eq. (1) diverge for $r \to 0$, the potential remains finite. Initially, we neglect variations of the penetration depth λ and the coherence length ξ due to thermal fluctuations on the microscopic scale and therefore we limit ourselves to temperatures far from T_c. The potential V is therefore temperature independent.

The two-dimensional Fourier transform of the potential given in Eq. (1) reads

$$v(q^2) = L_z \frac{\Phi_0^2}{4\pi}\left(\frac{1}{1+\beta q^2} - \frac{1}{\kappa^2 + \beta q^2}\right), \tag{2}$$

where we use the distance between vortices in the square lattice $a_\square = \sqrt{\Phi_0/B}$ as a unit of length (corresponding unit of the wave vector is $a_\square^{-1}$). L_z is the sample width in the z direction, and

$$\beta \equiv \frac{B\lambda^2}{\Phi_0} = \frac{B}{H_{c1}}\frac{\ln\kappa}{4\pi} \tag{3}$$

is a dimensionless magnetic field. The potential decreases as $1/q^4$ in the ultraviolet [commonly, the potential Eq. (2) is approximated by a simpler cutoff form $\frac{1}{1+\beta q^2}\exp(-\frac{\beta}{\kappa^2}q^2)$,[6,9] within the NLL approach of Kogan and co-workers]. In a fourfold symmetric superconductor generally there are asymmetries on the scales ξ and λ. One therefore can consider following two terms:

$$w(q_x,q_y) = \left[1 + \eta\left(\frac{\beta q_x q_y}{\kappa^2 + \beta q^2}\right)^2 + \eta_1\left(\frac{\beta q_x q_y}{1+\beta q^2}\right)^2\right] v(q^2). \tag{4}$$

The asymmetry factor in the square brackets does not diverge for either large or small momenta. The vortex-vortex interaction potential at distances larger than the core size was derived from a microscopic model of the d-wave superconductor by Yang.[18] The potential depending on the single parameter η is obviously not the most general one, but it allows us to qualitatively model the physics of the structural phase transitions in low-T_c superconductors, and in most of our calculations we use only this term.

In the framework of the London model, quenched disorder is described by a pinning potential (generated by all the pinning centers[19]) acting on each vortex,

$$E_{dis} = \frac{\Phi_0^2}{16\pi^2\lambda^2}\sum_a U(\mathbf{r}_a), \tag{5}$$

with the variance of the random potential assumed to be Gaussian (white noise) and short range,

$$\overline{U(\mathbf{r})U(\mathbf{r}')} = K(\mathbf{r}-\mathbf{r}') \propto \exp(-|\mathbf{r}-\mathbf{r}'|^2/\xi^2). \tag{6}$$

The Fourier transform of the correlator $\mathbf{K}(\mathbf{r}) = \Sigma_{BZ} K(q)\exp(i\mathbf{qr})$ in our units is

$$K(q) = \rho \exp\left(-\frac{\beta q^2}{\kappa^2}\right). \tag{7}$$

Expressions for the value of the material parameter ρ for the δT_c and the δl disorder in terms of the microscopic BCS parameters are given in Ref. 19. Here we regard the pinning strength constant ρ as a phenomenological parameter.

B. Vortex lattice structure in the presence of disorder

In this subsection we calculate perturbatively the influence of quenched disorder on the mesoscopic scale. We consider first the two-dimensional disorder system. It has two major realizations. The first is very thin films in which the vortex lines are stiff enough and do not bend significantly within the film. In this case the disorder (even the pointlike one) just displaces the vortices. The second is that of a thick sample in which columnar defects are present and their direction coincides with that of the magnetic field. Disorder generally pins the lattice leading to glassy dynamics and broadens the Bragg peaks, which eventually disappear in the vortex glass phase.[20]

The vortex lattice structure in clean materials is determined by the minimization of the lattice sum over the reciprocal lattice of arbitrary symmetry:

$$E_0 = \frac{1}{2}\sum_{a\neq b} W(\mathbf{r}_a - \mathbf{r}_b) = \frac{1}{2}\sum_{nm} w(\mathbf{G}_{nm}), \tag{8}$$

where $\mathbf{G}_{nm}$ are the reciprocal-lattice vectors. We restrict ourselves to rhombic lattices with the opening angle 2θ. It turns out that for a positive asymmetry parameter η, the rhombic lattices oriented along the crystallographic axis [110] with

$$\mathbf{G}_{nm} = n\mathbf{q}_1 + m\mathbf{q}_2; \quad \mathbf{q}_1 = \frac{1}{\sqrt{2\tan\theta}}(1,\tan\theta);$$

$$\mathbf{q}_2 = \frac{1}{\sqrt{2\tan\theta}}(1,-\tan\theta)$$

have lower energy than other lattice structures (rhombic oriented along [100] or oblique). Calculating the $E_0(\theta)$ sum for the rhombic lattices in the whole range of angles ($\theta = 45°-60°$), one finds out that above a certain critical asymmetry $\eta_c(\beta)$ the square lattice has lower energy than the rhombic, while below it one of the rhombic structures is preferred. The dependence of η_c on the magnetic field β in absolutely clean material is presented in Fig. 1. The value of the Ginzburg-Landau parameter is taken as $\kappa=5.6$ in all the simulations below. This value is typical for low-T_c tetragonal materials like those of the borocarbide family. Note that as β becomes large the fourfold anisotropy parameter approaches an asymptotic value $\eta_c^*=0.225$. For $\eta_c^* > \eta$ the lattice is always rhombic.

Pinning causes displacement of the vortices labeled by a from their equilibrium square lattice positions $\mathbf{R}_a$ by an amount $\mathbf{u}_a$. The energy $E[\mathbf{u}_a]$ of the displaced vortices is

$$E[\mathbf{u}_a] = \frac{1}{2}\sum_{a\neq b} W(\mathbf{R}_a - \mathbf{R}_b + \mathbf{u}_a - \mathbf{u}_b) + \sum_a U(\mathbf{R}_a + \mathbf{u}_a). \tag{9}$$

Expanding to second order in U and u (which leaves out third and higher orders in the disorder potential, neglected in the leading perturbative correction that we consider in this paper), one obtains

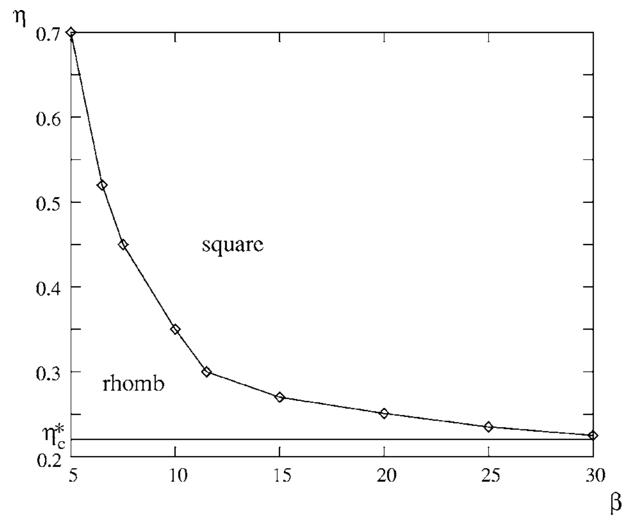

FIG. 1. The transition line in the clean case separating the rhombic vortex lattice phase from the square vortex lattice phase. The dependence of the critical fourfold anisotropy parameter η_c on dimensionless magnetic field $\beta=B\lambda^2/\Phi_0$. At large β it approaches an asymptotic value $\eta_c^*=0.225$ below which the lattice is rhombic for all fields. The Ginzburg-Landau parameter $\kappa=\lambda/\xi=5.6$.

$$\begin{aligned} E[\mathbf{u}_a] &= E_0 + \sum_a U(\mathbf{R}_a) + \frac{1}{2}\sum_{a\neq b} W'_\alpha(\mathbf{R}_a - \mathbf{R}_b)(\mathbf{u}_a^\alpha - \mathbf{u}_b^\alpha) \\ &+ \sum_a U'_\alpha(\mathbf{R}_a)\mathbf{u}_a^\alpha + \frac{1}{4}\sum_{a\neq b} W''_{\alpha\beta}(\mathbf{R}_a - \mathbf{R}_b)(\mathbf{u}_a^\alpha - \mathbf{u}_b^\alpha) \\ &\times (\mathbf{u}_a^\beta - \mathbf{u}_b^\beta). \end{aligned} \tag{10}$$

Switching to the Fourier harmonics on the Brillouin zone, $\mathbf{u}_a = \Sigma_{BZ} u_{\mathbf{q}}^\alpha \exp(i\mathbf{q}\mathbf{R}_a)$, $\mathbf{U}(\mathbf{r}) = \Sigma_{BZ} U_{\mathbf{q}} \exp(i\mathbf{q}\mathbf{r})$ one has

$$E[\mathbf{u}_q] = E_0 + \sum_{BZ} U_{\mathbf{q}} + \frac{1}{2}\sum_{BZ} \Lambda_{\alpha\beta}(q) u_{\mathbf{q}}^\alpha u_{-\mathbf{q}}^\beta + \sum_{BZ} iq_\alpha U_{\mathbf{q}} u_{\mathbf{q}}^\alpha. \tag{11}$$

Elastic moduli of the clean sample are given by the expansion of Λ to the second order in q: $\Lambda_{\alpha\beta}(q) = C^{\alpha\beta\gamma\delta} q_\gamma q_\delta$. The only nonzero moduli in the fourfold symmetry case are the compression C_{11}, the shear C_{66}, and C_{12}. A macroscopic manifestation of the structural phase transition is the softening of the elastic squash modulus,

$$C_{sq} = 2(C_{11} + C_{12}) - C_{66}, \tag{12}$$

at the transition point.[6] Note that C_{sq} vanishes for $\eta \to \eta_c$, while the other moduli are continuous across the transition line. The stability conditions (positively definite quadratic form $E_2[\mathbf{u_q}]$) for the square lattice are $4(C_{11}+C_{66}) > C_{sq} > 0$ and $C_{66} > 0$.

For a given lattice structure one generally obtains the displacement (strain) due to disorder,

$$u_{\mathbf{q}}^\alpha = \Lambda_{\alpha\beta}^{-1}(q) iq_\beta U_{\mathbf{q}}, \tag{13}$$

which when substituted into Eq. (11) leads to

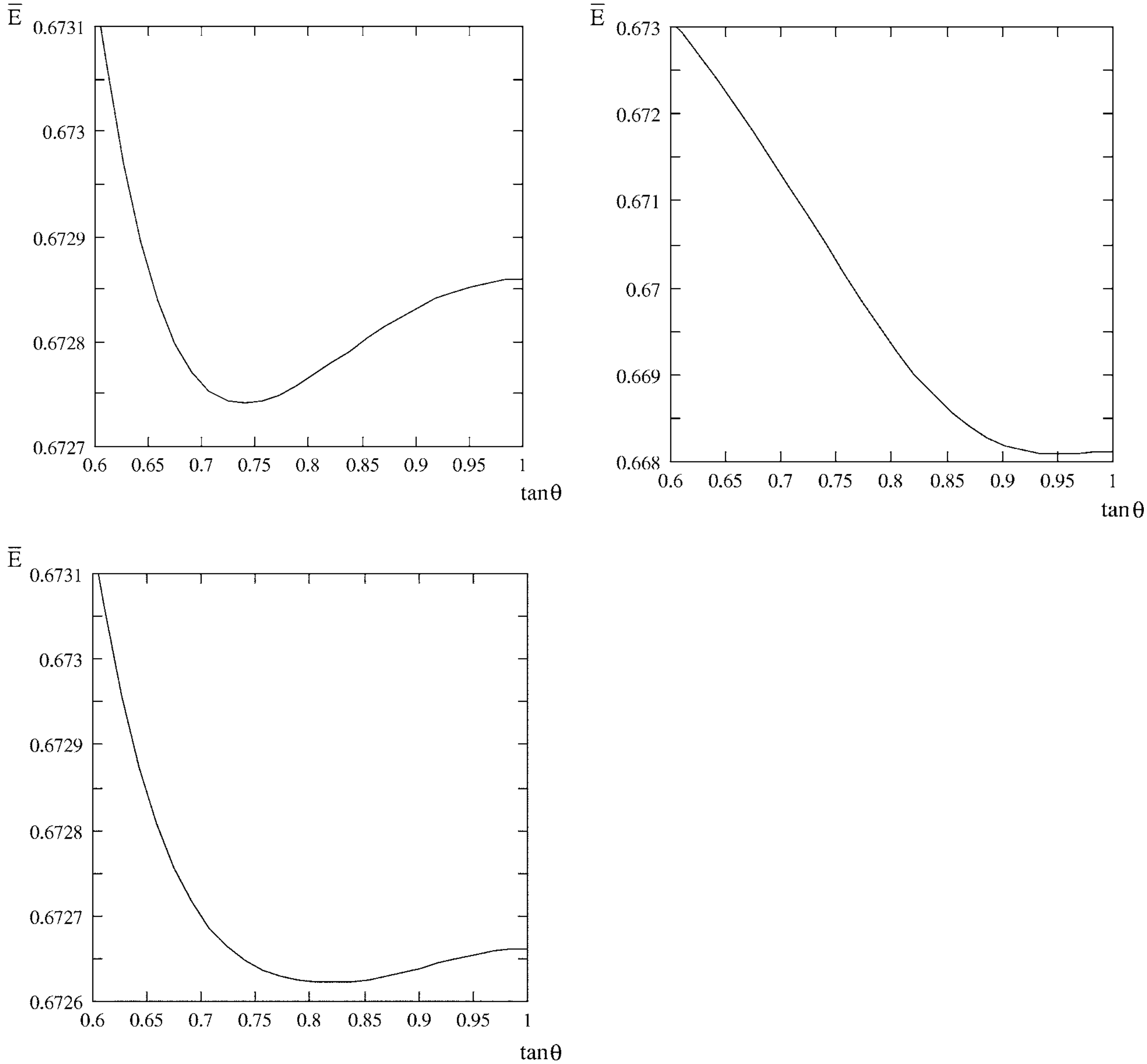

FIG. 2. The angular dependence of the vortex lattice energy for anisotropy parameter $\eta=0.22$ and dimensionless magnetic field $\beta=14$ and different pinning strengths. In the clean case for $\eta<\eta_c$ the lattice is rhombic. As the disorder strength increases the opening angle continuously approaches 90°. For (a) and $\rho=0$ the lattice is still rhombic, almost hexagonal, while for (b) $\rho=0.5$. It is already closer to square; (c) $\rho=11$ inside the square lattice phase.

$$E = E_0 + \sum_{BZ} U_{\mathbf{q}} - \frac{1}{2}\sum_{BZ} q_\alpha q_\beta \Lambda^{-1}_{\alpha\beta}(q) U_{\mathbf{q}} U_{-\mathbf{q}}. \tag{14}$$

Averaging over disorder, one obtains

$$\bar{E} = E_0 - \frac{1}{2}\sum_{BZ} \Lambda^{-1}_{\alpha\beta}(q) q_\alpha q_\beta K(q).$$

The total lattice energy was minimized numerically to determine the lattice structure with lowest energy, see Fig. 2, to be discussed below. These results can be generalized to the case of three-dimensional fourfold symmetric superconductor.

C. Lattice energy in the presence of pointlike disorder in the three-dimensional case

In this subsection we calculate perturbatively the influence of quenched disorder on the mesoscopic scale in the case of a three-dimensionsional fourfold symmetric superconductor. We therefore consider elastic lines (not necessarily stiff, but we will assume that the small tilt approximation[19] is applicable), of arbitrary length L_z and disorder which is localized in the field direction and arbitrary in the plane direction. The vortex lattice structure of the clean superconductor is still determined by minimization of E_0, Eq. (8), but now the pinning displaces lines from their equilibrium square lattice positions $\mathbf{R}_a$ by $\mathbf{u}_a(z) = \frac{1}{2\pi}\int_{q_z}\sum_{BZ} u^{\alpha}_{\mathbf{q}q_z} \exp(i\mathbf{q}\mathbf{R}_a + iq_z z)$. The variance of the random potential is assumed to be short range in the field direction,

$$\overline{U(\mathbf{r},\mathbf{z})U(\mathbf{r}',z')} = K(\mathbf{r}-\mathbf{r}')\delta(z-z').$$

The energy of displacements of vortices $\mathbf{u}_a$ is

$$E[\mathbf{u}_a(z)] = L_z E_0 + \int_{z=0}^{L_z} dz \left\{ \sum_a \left[\frac{\varepsilon}{2}\left[\frac{d\mathbf{u}_a(z)}{dz}\right]^2 + U(\mathbf{R}_a + \mathbf{u}_a(z),z) \right] + \frac{1}{2}\sum_{a\neq b} W[\mathbf{R}_a - \mathbf{R}_b + \mathbf{u}_a(z) - \mathbf{u}_b(z)] \right\}, \tag{15}$$

where ε is the line tension. Expanding to second order in U and u one has

$$E[\mathbf{u}_a] = L_z E_0 + \int_{z=0}^{L_z} dz \left\{ \sum_a \left[\frac{\varepsilon}{2}\left[\frac{d\mathbf{u}_a(z)}{dz}\right]^2 + U(\mathbf{R}_a,z) + U'_\alpha(\mathbf{R}_a,z)\mathbf{u}_a^\alpha(z) \right] + \frac{1}{4}\sum_{a\neq b} W''_{\alpha\beta}(\mathbf{R}_a - \mathbf{R}_b) \times [\mathbf{u}_a^\alpha(z) - \mathbf{u}_b^\alpha(z)][\mathbf{u}_a^\beta(z) - \mathbf{u}_b^\beta(z)] \right\}. \tag{16}$$

Using Fourier transform $\mathbf{U}(\mathbf{r},\mathbf{z}) = \Sigma_{BZ} U_{\mathbf{q}q_z} \exp(i\mathbf{q}r + iq_z z)$ one obtains

$$E[\mathbf{u}_q] = L_z E_0 + \frac{1}{2\pi}\sum_{BZ}\int_{q_z} dq_z \left(\frac{\varepsilon q_z^2}{2} u^\alpha_{\mathbf{q}q_z} u^\alpha_{\mathbf{q}q_z} + U_{\mathbf{q}q_z} + iq_\alpha U_{\mathbf{q}q_z} u^\alpha_{-\mathbf{q},-q_z} + \frac{1}{2}\Lambda_{\alpha\beta}(q) u^\alpha_{\mathbf{q}q_z} u^\beta_{-\mathbf{q},-q_z} \right). \tag{17}$$

For a given lattice structure one generally obtains the displacement (strain) due to disorder,

$$u^\alpha_{\mathbf{q}q_z} = [\Lambda_{\alpha\beta}(q) + \varepsilon q_z^2 \delta_{\alpha\beta}]^{-1} iq_\beta U_{\mathbf{q}q_z}, \tag{18}$$

which when substituted into Eq. (11) leads to

$$E = L_z E_0 + \frac{1}{2\pi}\sum_{BZ}\int_{q_z} dq_z \left(U_{\mathbf{q}q_z} - \frac{1}{2}[\Lambda_{\alpha\beta}(q) + \varepsilon q_z^2 \delta_{\alpha\beta}]^{-1} \times q_\alpha q_\beta U_{\mathbf{q}q_z} U_{-\mathbf{q},-q_z} \right). \tag{19}$$

Averaging over disorder one obtains

$$\bar{E} = E_0 - \frac{1}{4\pi}\sum_{BZ}\int_{q_z} dq_z \{[\Lambda_{\alpha\beta}(q) + \varepsilon q_z^2\delta_{\alpha\beta}]^{-1} q_\alpha q_\beta K(q)\}$$
$$= E_0 - \frac{1}{4\sqrt{\varepsilon}}\sum_{BZ} \{[\Lambda(q)]^{-1/2}_{\alpha\beta} q_\alpha q_\beta K(q)\}. \tag{20}$$

This should be minimized to obtain the lattice with lowest energy.

D. Phase diagram

Typical angular dependence of the lattice energy for different strengths of disorder is presented in Fig. 2. Both the anisotropy parameter η and the magnetic field are held constant. The second-order square-to-rhombohedral transition is clearly demonstrated. While Fig. 2(a) shows nearly hexagonal rhombic lattice, Fig. 2(b) exhibits nearly square rhombic and Fig. 2(c) has a minimum for the square lattice. Therefore as the disorder strength increases one crosses over into the square lattice phase. To analyze it we plotted the dependence of the anisotropy at which the square-to-rhombohedral transition takes place in the clean case as a function of magnetic field $\eta_c(\beta)$ in Fig. 1. There exists η_c^* such that for $\eta < \eta_c^*$ the lattice is rhombic for all fields. In this case, shown in Fig. 3(a) for $\eta = 0.22 < \eta_c^* = 0.225$, disorder induces a transition into the square lattice with $\beta_c(\rho)$ such that $\beta_c(\rho \to 0) \to \infty$. On the other hand for $\eta > \eta_c^*$ the limit is finite $\beta_c(\rho \to 0) \to \beta_c(\eta)$, see Fig. 3(b) for $\eta = 0.27$. Clearly in all cases for larger disorder the square phase appears at lower magnetic field. Up to now we have not considered the temperature dependence of the pinning strength.

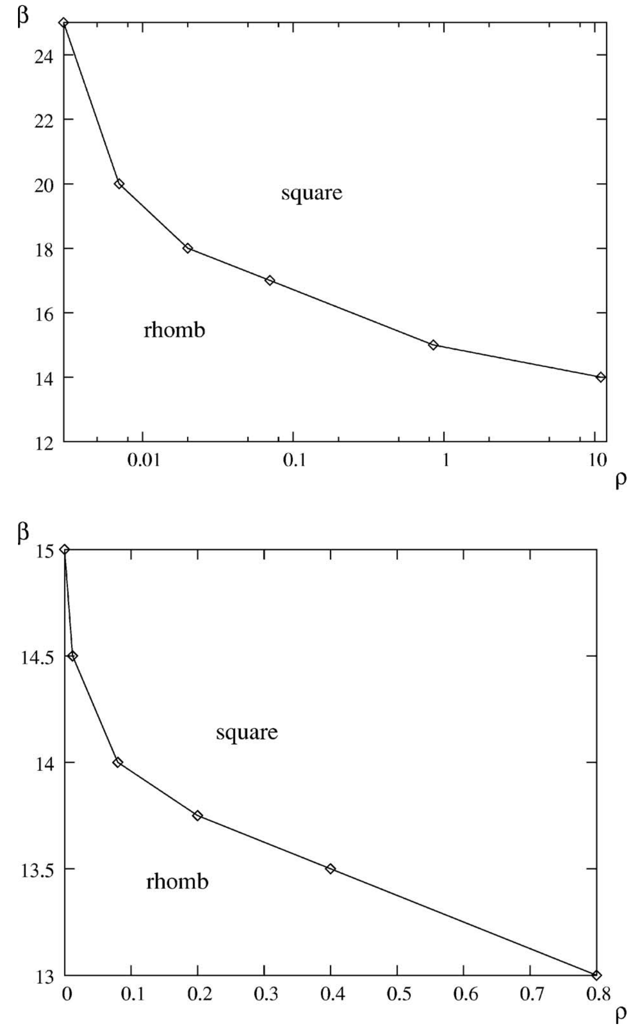

FIG. 3. The square-to-rhombohedral phase transition line in the pinning strength—magnetic field ($\rho-\beta$) space. For larger disorder the square phase appears at lower magnetic field. The shape of the line is qualitatively different in two cases (see text): low and high fourfold anisotropy: (a) $\eta = 0.22 < \eta_c^* = 0.225$. For $\eta < \eta_c^*$, the rhombic lattice always prevails and the square phase appears only for extremely large pinning strength. (b) $\eta = 0.27 > \eta_c^*$.

The pinning strength is strongly reduced as the temperature approaches the "thermal depinning" temperature

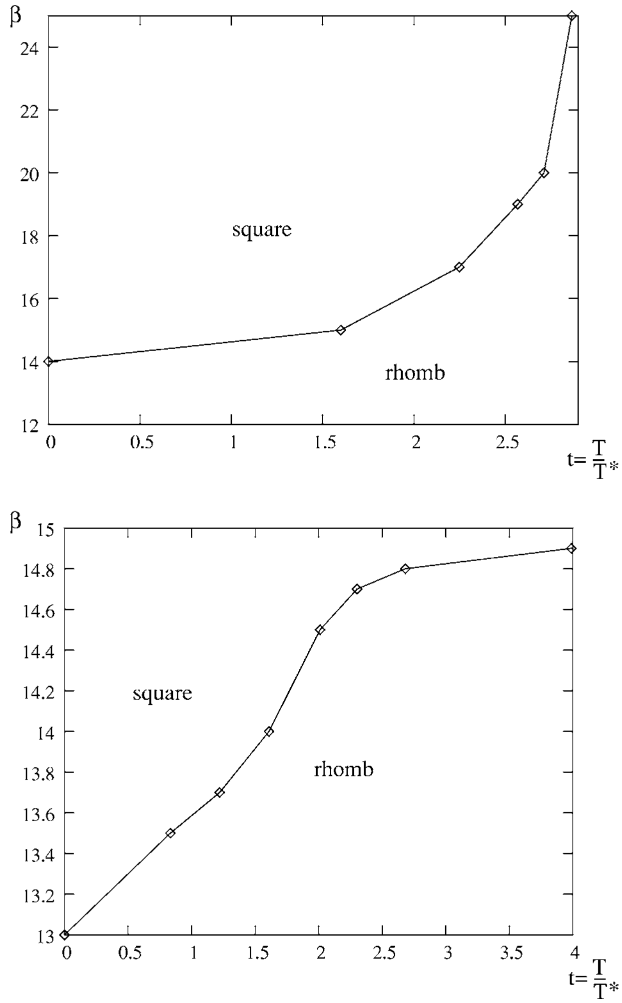

FIG. 4. T-B plane for fixed $\rho(0)$ in the nonlocal London approximation. The slope of the transition line is always positive. (a) $\eta=0.22<\eta_c^*=0.225$ for $\rho(0)=11$; (b) $\eta=0.27>\eta_c^*$ for $\rho(0)=0.8$.

$T^*\ll T_c$. The effect is believed to be exponential,[19]

$$\rho=\rho(0)\exp(-t^s), \tag{21}$$

where $t=T/T^*$. Neglecting weak dependence of the coherence and the penetration depth on temperature and anharmonicity effects, considered in Ref. 15 one can re-express the phase diagram in the B-T plane for fixed $\rho(0)$ and $s=2$, see Fig. 4. It is important to note that the slope of the transition line is positive, which is the main result of this paper. For $T<T^*$ the disorder is maximal and at $T=0$ $\beta_c=\beta_c[\rho(0)]$. Qualitatively the disorder effects are exponentially small for $T>T^*$ and the phase-transition line tilts sharply upwards for around $T=T^*$. At higher temperatures the two cases considered above are qualitatively different. While in the case $\eta<\eta_c^*$, β_c diverges at large T, see Fig. 4(a), in the $\eta>\eta_c^*$ case it approaches a finite value for a clean system value determined by $\eta=\eta_c(\beta)$, see Fig. 4(b). The former case might explain the upward tilt of the transition line observed in some experiments,[2] although one should exercise caution with such an interpretation within the framework of the London model. Experimentally the tilt occurs near the $H_{c2}(T)$ line. The London approach is valid as long as the magnetic field is far from $H_{c2}(T)$. In most experiments on both low-T_c and high-T_c superconductors a significant part of the data is taken in the region in which this requirement is not fulfilled. A way to describe the structural transformations of the vortex lattice is to resort to the Ginzburg-Landau approach valid far from $H_{c1}(T)$.

III. GINZBURG-LANDAU APPROACH

When fields of vortices overlap $[H_{c1}(T)\ll B]$, the magnetic induction is nearly constant. The Ginzburg-Landau (GL) approach is a good approximation for strongly type-II superconductors (borocarbide superconductors with $\kappa \sim 10-20$ belong to this class) in a wide range of fields. Within this approximation the kinetic energy of supercurrents (the largest contribution to the total energy) and the energy associated with gradients of the modulus of the order parameter (core-core interactions between vortices is a part of it) are both included on an equal footing.

A. Anisotropic Ginzburg-Landau functional with quenched disorder

Near T_c the system is phenomenologically described by the GL free-energy functional of the appropriately rescaled order-parameter field ψ (note that we use the coherence length as the unit of length, which is smaller than the unit of length in the London model in previous sections by factor $\sqrt{2}\pi$; details can be found in Refs. 7 and 8):

$$\frac{F_{GL}}{T_c}=\frac{1}{\sqrt{2Gi}\pi^2}\int d^3x\left(\psi^*\mathcal{H}\psi-a_h|\psi|^2+\frac{1}{2}|\psi|^4\right), \tag{22}$$

where the Ginzburg number, a dimensionless parameter characterizing the strength of thermal fluctuations, is

$$Gi\equiv\frac{1}{2}\left(\frac{32\pi e^2\kappa^2\xi T_c\gamma}{c^2h^2}\right)^2, \tag{23}$$

with the effective-mass anisotropy $\gamma\equiv\sqrt{m_c/m_{ab}}$ (related to the anisotropy of the coherence lengths in and out of the basal plane), and $a_h=\frac{1-t-b}{2}$, $b=B/H_{c2}$, $t=T/T_c$ (near T_c, when we take $H_{c2}=-T_c\frac{dH_{c2}(T)}{dT}$). In the present formalism, the superconducting order parameter ψ has only one (complex) component. Therefore a way to account for the fourfold symmetric but $O(2)$ rotation noninvariant (anisotropic) properties of the system is to include additional terms in the gradient part of the free energy. These terms should have at least four derivatives D^4 and fortunately there is only one combination like that. Of course one can always have rotation invariant gradient terms as well.

The gradient part of the free energy therefore has both isotropic and anisotropic parts[7] $\mathcal{H}=\mathcal{H}_0+\mathcal{H}'$:

$$\mathcal{H}_0=-\vec{D}^2-\partial_z^2=ba^\dagger a-\frac{1}{2}\partial_z^2,$$

$$\mathcal{H}' = -\frac{\tilde{\eta}}{4}\{\cos(4\Theta)[(D_x^2 - D_y^2)^2 - (D_xD_y + D_yD_x)^2] + \sin(4\Theta) \times[(D_x^2 - D_y^2)(D_xD_y + D_yD_x) + (D_xD_y + D_yD_x) \times(D_x^2 - D_y^2)]\} = -b^2\tilde{\eta}[(a^\dagger)^4 e^{4i\Theta} + a^4 e^{-4i\Theta}], \tag{24}$$

where Θ is the angle between the rhombic lattice and the atomic lattice and $D_x = \partial_x - iby$, $D_y = \partial_y$ and $\tilde{\eta}$ can be positive (usually in low-T_c materials) or negative (usually in high-T_c materials). It is convenient to express covariant derivatives in the directions perpendicular to the external applied field in terms of operators of creation and annihilation of Landau levels,

$$\hat{a}^\dagger \equiv -\frac{1}{\sqrt{2b}}(D_x - iD_y), \quad \hat{a} \equiv \frac{1}{\sqrt{2b}}(D_x + iD_y). \tag{25}$$

For convenience in Eq. (24) we have chosen a combination such that $\mathcal{H}'$ does not change the $H_{c2}(T)$ line produced by $\mathcal{H}_0$ (up to order of $\tilde{\eta}$).

The fourfold symmetric anisotropy within the basal plane of a particular material is described by a single phenomenological coefficient $\tilde{\eta}$. It is a constant within GL approach, but in fact it can depend (weakly) on temperature and other external parameters. For the vortex lattice, the effective magnitude of the fourfold anisotropy depends also on the magnetic induction and should be specified by a parameter that is proportional to $b\tilde{\eta}$.

To describe the disorder (pinning) potential one adds a random component $a_h W(\mathbf{r})|\psi(\mathbf{r})|^2$ to the term $a_h|\psi(\mathbf{r})|^2$, to the GL functional, Eq. (22). We assume that $W(\mathbf{r})$ has a Gaussian random distribution with variance,

$$\overline{W(\mathbf{r})W(\mathbf{r}')} = n\delta^{(3)}(\mathbf{r} - \mathbf{r}'), \tag{26}$$

n is a dimensionless constant and is assumed to be independent of temperature and magnetic field. It is related to the average number of pinning center per volume $\xi_{a,b}^2\xi_c$. The average of a quantity O which averages over the ensemble of realizations of the disorder is defined to be

$$\bar{O} = \frac{\int_a O[W(\mathbf{r})]\exp\{-\int d\mathbf{r}[W(\mathbf{r})^2/2n]\}}{\int_a \exp\{-\int d\mathbf{r}[W(\mathbf{r})^2/2n]\}}. \tag{27}$$

B. Structure of the vortex lattice in the clean case

In order to locate the $H_{c2}(T)$ line, one first solves the linearized GL equation $\mathcal{H}\psi = a_h\psi$. For $a_h < 0$ a nontrivial solution (different from $\psi = 0$) appears. In the present case of tetragonal symmetry, we have to study the eigenfunctions of a differential operator which differs from the standard one by the $\mathcal{H}'$ terms. The GL equation in a form that facilitates the solution by the expansion in $a_h = \frac{1-t-b}{2}$, the distance from H_{c2} line, can be written as

$$\mathcal{H}\psi - a_h\psi + \psi|\psi|^2 = 0, \tag{28}$$

$$\mathcal{H} = ba^\dagger a - \frac{1}{2}\partial_z^2 - b^2\tilde{\eta}[(a^\dagger)^4 e^{4i\Theta} + a^4 e^{-4i\Theta}]. \tag{29}$$

Assuming that $\eta^{GL} = \sqrt{3/2}b\tilde{\eta} \ll 1$, the anisotropic part of $\mathcal{H}'$ is treated as a perturbation, using standard perturbation theory for the Schrodinger equation. This means we expect that the presence of anisotropy modifies the eigenfunctions of the isotropic problem,

$$\varphi_{N,k}(x,y,z) = C_N e^{ik_z z}\sum_{l=-\infty}^{+\infty} H_N(x - \sqrt{\pi\tan\theta}l - k_y) \times\exp\{i[\pi\rho(l^2 - l) + \sqrt{\pi\tan\theta}l(y + k_x) + yk_y]\} \times\exp\left[-\frac{1}{2}(x - \sqrt{\pi\tan\theta}l - k_y)^2\right], \tag{30}$$

where $C_N = \sqrt{\frac{\sqrt{\tan\theta}}{2^N N!}}$. Here $\varphi_{N,k}(x,y,z)$ is normalized so that average of $|\varphi_{N,k}(x,y,z)|^2$ in a unit cell is equal to 1. To simplify the notation, from now on $\langle\cdots\rangle$ denotes the average over a unit cell in real space. These are the familiar Landau levels stacked into a rhombic lattice defined by half of the opening angle of the rhombic lattice θ and normalized. Thus we obtain a set of "shifted" Landau levels:

$$\phi_{Nk} = \varphi_{Nk} - b^2\tilde{\eta}\sum_{M\neq N}\frac{\langle\varphi_{M,k}|(a^\dagger)^4 e^{4i\Theta} + a^4 e^{-4i\Theta}|\varphi_{N,k}\rangle}{b(N-M)}\varphi_{Mk} + \cdots . \tag{31}$$

In what follows we employ the lowest Landau-level approximation in terms of these new functions that have the form

$$\phi_{0k} \equiv \phi_k = \varphi_k + \eta^{GL}e^{4i\Theta}\varphi_{4k}. \tag{32}$$

The solution to Eq. (28) has the form

$$\psi = \sqrt{a_h}(\Psi_0 + a_h\Psi_1 + \cdots),$$

$$\Psi_0 = c\phi_0, \quad \Psi_1 = \sum_N c_N\phi_N, \quad \cdots , \tag{33}$$

which is formally identical to the case of the isotropic GL model. We work in the lowest order of the a_h expansion.

The normalization coefficient c is fixed by the nonlinear terms of the HDGL equation:

$$c^{-2} = \langle|\phi_0|^4\rangle_{u.c.} \equiv B_0 \approx \langle|\varphi_0|^4\rangle + 2\eta^{GL}\,\mathrm{Re}(e^{4i\Theta}\langle\varphi_4\varphi_0^*|\varphi_0|^2\rangle) \equiv \beta_0 + 4\eta^{GL}\beta_4\cos(4\Theta),$$

$$\beta_0 = \langle|\varphi_0|^4\rangle, \quad \beta_4 = \langle\varphi_4\varphi_0^*|\varphi_0|^2\rangle, \tag{34}$$

where we used the fact that $\mathrm{Im}\,\beta_4 = 0$.

The mean-field free-energy density has the form

$$F_0(\theta) = -\frac{a_h^2}{2B_0(\theta)} + \mathcal{O}(a_h^3). \tag{35}$$

The quantity B_0 depends on the geometrical parameters θ and Θ of the vortex lattice. The minimization with respect to them determines the orientation and shape of the vortex lattice at equilibrium. For $\pi/4 < \theta < \pi/3$, we have $\beta_4 < 0$ and we obtain

$$F_0(\theta) = -\frac{a_h^2}{2}\frac{1}{\beta_0 + 4|\eta^{GL}|\beta_4} \quad (36)$$

as $\cos 4\Theta = \eta^{GL}/|\eta^{GL}|$ will minimize the free energy. Therefore for positive η^{GL}, $\Theta=0$ and for negative η^{GL}, $\Theta=\pi/4$. The minimization with respect to θ was performed numerically in Ref. 7. The phase transformation between the square and rhombic lattices found in this way is continuous. Therefore in order to find the boundary between these phases it is also possible, and more convenient in this case, to study the conditions for the stability of the more symmetric square phase. The condition for stability reads

$$\left.\frac{d^2F_{mf}(\theta)}{d\theta^2}\right|_{\theta=\pi/4} = 0 \quad (37)$$

or

$$\beta_0''\left(\theta=\frac{\pi}{4}\right) + 4|\eta_c^{GL}|\beta_4''\left(\theta=\frac{\pi}{4}\right) = 0 \quad (38)$$

which yields $|\eta_c^{GL}|=0.029\,23$, i.e., the phase-transition line b_{SPT}:

$$b_{SPT} = \frac{0.023\,87}{|\tilde{\eta}|}.$$

In this approximation the line of square-rhombohedral structural phase transformation (SPT line) is parallel to the temperature T axis. Note, however, that some (weak) temperature dependence can appear through the parameter $\tilde{\eta}$.

The small magnitude of η_c^{GL} means that the SPT occurs well below $H_{c2}(T=0)$ and justifies our approach in which in $\mathcal{H}$ of Eq. (24) $\mathcal{H}'$ is treated as a perturbation. We now calculate the corrections to the mean-field free energy of Eq. (36) due to weak disorder, and then find corrections to the SPT line.

C. Effect of weak disorder

If a weak potential profile (disorder potential) is present in the system then the vortex lattice distorts to take advantage of the places where the local T_c (at given magnetic field H) is higher and to avoid the places with lower T_c. The complete energy reads

$$F = F_0(W=0) + F_{dis}. \quad (39)$$

The method to take into account the disorder that we employed and the details of the derivation of the following Eq. (40) are given in the Appendix. Neglecting thermal fluctuation in this case we find the mean-field free-energy density of the vortex lattice receives a negative corrections which has the form

$$F_{dis} = -\frac{a_h^2\sqrt{a_h}n}{B_0 8\sqrt{2}\pi^2}\int_{BZ} d^2k\left(\frac{B_k - |G_k|}{\sqrt{\epsilon_k^A}} + \frac{B_k + |G_k|}{\sqrt{\epsilon_k^O}}\right), \quad (40)$$

with

$$B_k = \langle|\phi_0|^2\phi_k\phi_k^*\rangle, \quad G_k = \langle(\phi_0^*)^2\phi_{-k}\phi_k\rangle_{u.c.}.$$

The phonon spectrum dispersion functions ϵ_k^A and ϵ_k^O are

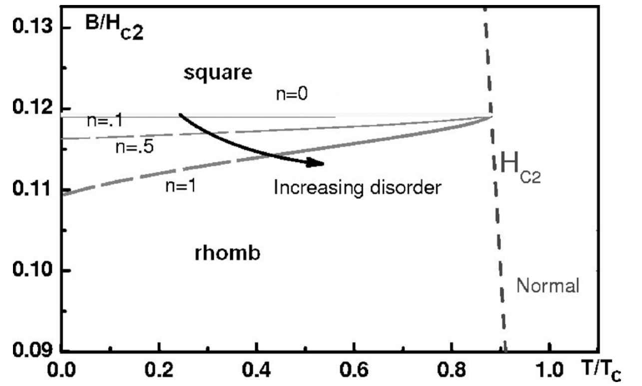

FIG. 5. Ginzburg-Landau model with the four derivative asymmetric term with asymmetry parameter $\eta^{GL}=0.2$. Square-to-rhombohedral transition line for different dimensionless disorder strength n. The slope of the line is positive and increases with pinning strength.

$$\epsilon_k^A = \frac{2}{B_0}B_k - 1 - \frac{1}{B_0}|G_k|, \quad (41)$$

$$\epsilon_k^O = \frac{2}{B_0}B_k - 1 + \frac{1}{B_0}|G_k|. \quad (42)$$

The energy of the acoustic branch vanishes at $\mathbf{k}=0$ since they are the Goldstone bosons associated with disappearance of the continuous translation symmetry at the homogeneous-vortex lattice transition. Note that expanding in η^{GL} preserves the property $\epsilon_{k=0}^A=0$.

The location of the SPT line is now obtained by minimization of the corrected free energy Eq. (40). The results for several values of the disorder strength are given in Fig. 5. The square-to-rhombohedral transition line for different dimensionless disorder strength n is defined by $R=n\xi_{ab}^2\xi_c$. One observes again that the slope is positive.

IV. DISCUSSION AND CONCLUSIONS

While in high-T_c superconductors like LaSCO the slope of the rhombohedral-to-square transition line in the T-H plane is negative,[13,15] in low-T_c superconductors it can be positive. We demonstrated here that the influence of the pointlike quenched disorder rather than thermal fluctuations is responsible for this feature. Both the nonlocal London (NLL) and the anisotropic (containing a four derivative fourfold symmetric term) Ginzburg-Landau model's calculations with disorder incorporated support the general argument that the more symmetric square lattice gains energy over the less symmetric rhombic one. The difference stems from the fact that the disorder strength diminishes at higher temperatures due to thermal depinning. Consequently both the NLL at low temperatures and HDGL at high temperatures lead to a positive slope of the transition line, see Figs. 4 and 5. This tendency is opposite to the influence of thermal fluctuations considered in Ref. 15 in which we argued that thermal fluctuations in the clean case favor the square phase. Combining the results of the two models with parameters appropriate to

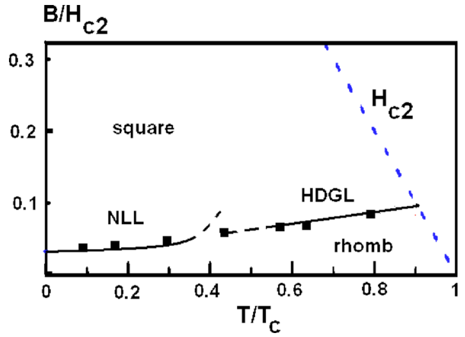

FIG. 6. (Color online) Square-to-rhombohedral transition line incorporating both the nonlinear London model and the anisotropic Ginzburg-Landau one. Squares are experimental data of Ref. 5.

YNi_2B_2C one can describe the results of a recent experiment,[5] see Fig. 6.

Several comments are in order. The difference between strongly "fluctuating" high-T_c materials like LaSCO and YBCO (and some layered low-T_c materials) and most of the low-T_c materials like borocarbides is in the relative importance of thermal fluctuations on the mesoscopic scale and disorder. While in high-T_c materials the thermal fluctuations are dominant, in low-T_c ones the quenched disorder is dominant in determining the structure of the vortex lattice. One concludes therefore that materials with strong thermal fluctuations exhibit a negative slope of structural phase transition line (at least well below the melting line). When thermal fluctuations are small and disorder prevails one expects a positive slope.

Note that in this paper we assumed that the disorder correlator is rotationally symmetric, see Eqs. (6) and (26), in NLL and HDGL models, respectively. This is not always the case.[24] The origin of the fourfold symmetric terms in phenomenological models breaking the full $O(2)$ invariance in the ab plane is the coupling between the vortex lattice and the atomic lattice. This in turn originates on the microscopic level from two somewhat related anisotropies: the Fermi velocity dependence on the angle and the anisotropy of the gap function.[25–27] Similarly the disorder can be correlated on the microscopic or mesoscopic scale. For example, twinning planes oriented along $[1\bar{1}0]$, $[\bar{1}10]$ directions will obviously cause the disorder correlator [see Eq. (6)] to be fourfold symmetric rather than rotationally invariant correlator

$$K(\mathbf{q}) = K_i(|q|) + \cos(4\phi)K_a(|q|),$$

where ϕ is the polar angle of $\mathbf{q}$. This would produce an effect different from the one produced by the rotationally invariant case.

Note also that square-to-rhombohedral transition is not limited to nonmagnetic borocarbides YBCO and LSCO. Some other examples include $CeCoIn_5$,[22] and V_3Si.[21] Recently Glover and co-workers[24] developed a method to determine the structural transition line from the tilt angle dependence of the corresponding peak effect.[15,23]

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APPENDIX

In this Appendix we provide some details of the calculation of the free energy in the GL approach. The free-energy density averaged over disorder can be represented (using the GL equation) as follows:

$$F = -\frac{1}{2}\overline{\langle|\psi(\mathbf{r};W)|^4\rangle_{u.c.}} = F_0 + \overline{F_{dis}},$$

where F_0 is independent of disorder.

The free-energy correction of the GL equation is $a_h W(x)|\psi|^2$. The magnitude of the disorder is characterized by n appearing in the disorder correlator $\overline{W(x)W(y)} = n\delta^{(3)}(\mathbf{r}-\mathbf{r}')$. It is convenient to introduce a new random potential $U(\mathbf{r}) = W(\mathbf{r})/\sqrt{n}$ with the correlator $\overline{U(\mathbf{r})U(\mathbf{r}')} = \delta^{(3)}(\mathbf{r}-\mathbf{r}')$. We rewrite the HDGL Eq. (28) as

$$\mathcal{H}\psi - a_h\psi + \psi|\psi|^2 + a_h\gamma U(\mathbf{r})\psi = 0, \tag{A1}$$

where we introduced the new perturbation parameter $\gamma = \sqrt{n}$.

Expanding in γ, one gets

$$\psi(\mathbf{r};U) = \sqrt{a_h}\left[\Psi_0 + \sum_{m=1}^{m}\gamma\Psi_m\right]. \tag{A2}$$

The first term is given by the linearized GL equation: $\Psi_0 = c\phi_0$ with $c = 1/\sqrt{B_0}$. The equations for the next two terms are

$$\left(1 - \frac{1}{2a_h}\partial_z^2 - 2|\Psi_0|^2\right)\Psi_1 - \Psi_0^2\Psi_1^* = U\Psi_0,$$

$$\left(1 - \frac{1}{2a_h}\partial_z^2 - 2|\Psi_0|^2\right)\Psi_2 - \Psi_0^2\Psi_2^* = 2|\Psi_1|^2\Psi_0 + \Psi_1^2\Psi_0^* + U\Psi_1. \tag{A3}$$

The unknown functions are found using the expansion in ϕ_k basis: $\Psi_1 = \int_k d_k\phi_k$, $\Psi_2 = \int_k e_k\phi_k$. The coefficients of these expansions read

$$d_0 = -\frac{c}{2}U_0,$$

$$d_k = \frac{c}{\Delta_k}\left[\left(1 - 2\frac{B_k}{B_0} - \frac{k_z^2}{2a_h}\right)U_k + \frac{G_k^*}{B_0}U_{-k}^*\right], \quad k \neq 0, \tag{A4}$$

$$e_0 = -\frac{1}{2c}\int_k |d_k|^2,$$

$$\Delta_k = \left[2\frac{B_k}{B_0} - 1 - \frac{|G_k|}{B_0} + \frac{k_z^2}{2a_h}\right]\left[2\frac{B_k}{B_0} - 1 + \frac{|G_k|}{B_0} + \frac{k_z^2}{2a_h}\right], \tag{A5}$$

where $U_k = \langle U(\mathbf{r})\phi_k^*(\mathbf{r})\phi_0(\mathbf{r})\rangle_{u.c.}$. The coefficients e_k with $k \neq 0$ are not needed for our purposes.

The correction to the free-energy density due to disorder is given by

$$\begin{aligned}\overline{F_{dis}} &= -\frac{a_h^2\gamma^2}{2(2\pi L_z)}\int_x \{4\overline{|\Psi_1|^2}|\Psi_0|^2 + [2\overline{\Psi_2^*}\Psi_0|\Psi_0|^2 + \overline{(\Psi_1^*)^2}\Psi_0^2 \\ &\quad + \text{c.c.}]\} = -\frac{a_h^2\gamma^2}{2}\left\{4c\overline{e_0} + \int_k\left[4\frac{B_k}{B_0}\overline{|d_k|^2}\right.\right. \\ &\quad \left.\left. + \left(\frac{G_k^*}{B_0}\overline{d_k d_{-k}} + \text{c.c.}\right)\right]\right\} \\ &= -\frac{a_h^2\gamma^2}{2}\int_k\left[-2|d_k|^2 + 4\frac{B_k}{B_0}\overline{|d_k|^2} + \left(\frac{G_k^*}{B_0}\overline{d_k d_{-k}} + \text{c.c.}\right)\right] \\ &= \frac{a_h^2\gamma^2}{2}c\int_k(\overline{d_k^* U_k} + \text{c.c.}).\end{aligned} \tag{A6}$$

At the last step the equation for d_k has been used. Performing disorder averages we obtain

$$\begin{aligned}\overline{F_{dis}} &= \frac{a_h^2\gamma^2 c}{2}\int_k(\overline{d_k^* U_k} + \text{c.c.}) \\ &= \frac{a_h^2\gamma^2}{2}c\left\{\int_k\frac{1}{\Delta_k}\left[\left(1 - 2\frac{B_k}{B_0}\right)\overline{U_k U_k^*}\right.\right. \\ &\quad \left.\left. + \frac{G_k}{B_0}\overline{U_k^* U_{-k}^*} + \text{c.c.}\right]\right\} \\ &= \frac{a_h^2\gamma^2}{2}c^2\left\{\int_k\frac{1}{\Delta_k}\left[\left(1 - 2\frac{B_k}{B_0}\right)B_k + \frac{G_k}{B_0}G_k^*\right]\right\} \\ &= -\frac{a_h^2\gamma^2}{2}\left(\int_k\frac{B_k - |G_k|}{2B_k - B_0 - |G_k| + B_0 k_z^2/2a_h}\right. \\ &\quad \left. + \int_k\frac{B_k + |G_k|}{2B_k - B_0 - |G_k| + k_z^2 B_0/2a_h}\right).\end{aligned}$$

Performing the k_z integration we arrive at the formula Eq. (40) in which the numerator was expressed via dispersion relations.

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