Effect of fluctuations on vortex lattice structural transitions in superconductors

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The rhombic-to-square transition field $H_c(T)$ for cubic and tetragonal materials in fields along [001] is evaluated using the nonlocal London theory with account of thermal vortex fluctuations. Unlike extended Ginzburg-Landau models, our approach shows that the line $H_c(T)$ and the upper critical field $H_{c2}(T)$ do not cross due to strong fluctuations near $H_{c2}(T)$ which suppress the square anisotropy induced by the nonlocality. In increasing fields, this causes re-entrance of the rhombic structure in agreement with recent neutron scattering data on borocarbides.

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Complex behavior of vortex lattices (VLs) even in cubic superconductors like Nb has been known for a long time [1]. Recent progress in understanding the evolution of VLs with the magnetic field $H$ and temperature $T$ became possible due to availability of large high quality crystals of borocarbides [2], which triggered a score of small-angle neutron scattering (SANS) [3,4], scanning tunneling [5,6], and decoration experiments [7]. Of a particular interest is the ubiquitous structural transition between rhombic and square VLs in increasing fields along the $c$ axis of tetragonal borocarbides [8].

For this case, the vortex repulsion is isotropic within the standard London and Ginzburg-Landau (GL) theories, so that vortices should always form the hexagonal Abrikosov lattice, which provides the maximum vortex spacing for a given flux density $\phi_0/(2\pi B)$, where $\phi_0$ is the flux quantum. There is no coupling between the VL and the crystal in these models; as a consequence, the VL orientation is arbitrary and no VL structural transitions are expected. A full microscopic theory of the mixed state contains this coupling, but involves self-consistent calculations of the gap and current distributions, a formidable task even for materials with the GL parameter $\lambda^2 T_\text{c} \sim 1$ [1].

The situation simplifies in high-$\kappa$ materials (like borocarbides), for which one can utilize a more transparent nonlocal London model [10]. Within this approach, the VL coupling to the crystal is provided by the basic nonlocal relation between the current density and the vector potential, $J_\alpha(r) = \int Q_{\alpha\beta}(r-r')A_\beta(r')d^3r'$, where the kernel $Q$ depends on the Fermi surface [10], the pairing symmetry [12], and the field orientation. Here, we consider cubic or tetragonal s-wave materials in fields along the $c$ axis so that $Q(r)$ has the square symmetry.

The kernel $Q(r)$ decays over the nonlocality range $\rho = f(T, \ell)/\xi_0$ so that $\ell$ is the mean-free path for nonmagnetic scatterers and $\xi_0$ is the BCS zero-$T$ coherence length. The function $f$ decreases slowly with $T$ and is suppressed strongly by scattering [10]. The nonlocality adds to the intervortex interaction a short-range potential $V(x,y)$ with the symmetry of the crystal. In the low field limit, $V$ is irrelevant and the VL is triangular; still, $V$ removes the orientational degeneracy and locks the VL onto certain crystal direction. With decreasing intervortex spacing $a(B)$, the potential $V$ drives the triangular VL into a square at a field $H_c(T)$. The transition curve $H_c(T)$ is the subject of this work.

The nonlocal London model describes correctly the observed structure and orientation of rhombic VLs in small fields [5] and the structural evolution toward the square [8]. Moreover, the fast increase of $H_c$ with increasing impurity concentration predicted by the model has been verified by SANS [13]. Still, there is an open question on what happens when the applied field $H > H_c$ keeps increasing.

Below we evaluate the mean-squared amplitude of thermal vortex fluctuations using the elastic energy of the deformed VL. Unlike the case of isotropic superconductors, an important role in this energy is played by VL rotations relative to the crystal. We show that $V$ remains finite at the transition line $H_c(T)$, but diverges as $B$ approaches $H_{c2}(T)$. In the vicinity of $H_{c2}(T)$, the
anisotropic nonlocal potential $V(x, y)$ is averaged out by fluctuations, and the interaction becomes isotropic.

As a result, the rhombic VL becomes preferable, turning into the hexagonal Abrikosov VL as $B \rightarrow H_{c2}$. The re-entrance of the rhombic VL in increasing fields occurs if $u^2 \sim \xi_0^2$, i.e., the amplitude of fluctuations needed to wash out the nonlocal effects is much smaller than that required for the VL melting. This re-entrance, therefore, can happen in nearly cubic materials, in which vortices are not split into “pancakes” and fluctuations are weak. We evaluate the shape of the $H_c(T)$ curve using model parameters of LuNi$_2$B$_2$C for which in the clean limit $\rho(T) \approx (1/2)\xi_0$. We reproduce the shape of this curve seen in the SANS data [10]. We take all moduli in Eq. (1) except the tilt modulus $c_{44}$ as practically nondispersive [18].

Next, we calculate the mean-squared vortex displacement $\langle \mathbf{u}^2 \rangle = \overline{u_x^2} + \overline{u_y^2}$, where $u_x$ and $u_y$ are the amplitudes of displacement fluctuations in $x$ and $y$ directions, respectively. The shear energy depends on the shear direction, but the corresponding moduli can all be expressed in terms of $c_x$ and $c_{\omega}$ [19]. We take all moduli in Eq. (1) except the tilt modulus $c_{44}$ as practically nondispersive [18].

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Here, \( p = [\pi C + \chi(T)\eta(t,b)/s(b)]=, g = m^2 + n^2, d = \mu + g + \zeta(b)(m^2 - n^2)^2, \mu = 1/2\pi bk^2 \). The dimensionless control parameters \( \chi \) and \( \zeta \) quantify the amplitude of thermal displacements and the nonlocal corrections:

\[
\chi = \frac{16\sqrt{2}\pi^3 \lambda_0 \lambda cT}{\phi_0^2 \xi_0}, \quad \zeta = \frac{\pi}{2} \left( \frac{\rho}{\xi} \right)^2.
\]  

(8)

Note that nonlocality enters also the exponent \( p \) in Eq. (8) via the parameter \( \eta \).

For the further analysis, we assume that \( \lambda(T) = \lambda(0)/(1 - t^2)^{1/2} \) and \( \xi(T) = \xi(0)/(1 - t^2)^{1/2} \), where \( t = T/T_c \) (qualitatively, our results do not change if other plausible \( T \) dependences are used). Then

\[
\chi = \chi_0 t \sqrt{1 - t^2}, \quad \zeta = \zeta_0 (1 - t^2),
\]

(9)

\[
\lambda_0 = \frac{16\sqrt{2}\pi^3 \lambda_0(0) \lambda_c(0) T_c}{\phi_0^2 \xi_0(0)}, \quad \zeta_0 = \frac{\pi}{2} \left( \frac{\rho}{\xi_0} \right)^2.
\]

(10)

In the clean limit \( \zeta_0 \sim 1 \); with increasing scattering, \( \zeta_0(\ell) \) drops fast. For \( \text{LuNi}_2\text{B}_2\text{C} \) with \( T_c = 16 \text{ K} \), \( \zeta_0 \approx 70 \text{ Å} \), \( \lambda_0(0) \approx 10^4 \text{ Å} \), and \( \lambda_c(0) \approx 1.2 \times 10^4 \text{ Å} \), we estimate \( \chi_0 \approx 6.4 \times 10^{-3} \ll 1 \). The smallness of \( \chi_0 \) indicates that fluctuations contribute little to the thermodynamics of stable VLs. As shown below, being crucial on the upper branch of \( H_{\parallel}(T) \), fluctuations are negligible on the lower branch.

Strictly speaking, \( H_{\parallel}(T) \) should be calculated self-consistently taking into account the effect of fluctuations on the relevant moduli. However, since \( u^2 \) is finite at \( H_{\parallel} \), we may neglect the thermal softening of \( c_x \) and \( c_w \). Then, \( H_{\parallel}(T) \) is just a root of Eqs. (4), which we find numerically. The factor \( \eta \) which enters \( p \) in Eq. (8) is a much weaker function of \( t \) and \( b \) than \( \chi(t)/s(b) \) (\( \eta \) varies from 1.6 for \( c_w/c_x = 1 \) to 3 for \( c_w/c_x = 0.1 \)). For this reason we disregard variation of \( \eta \), adopting \( \eta = 2.7 \) for \( \text{LuNi}_2\text{B}_2\text{C} \) with \( c_w/c_x \sim 0.2 \) at \( H_{\parallel} \.

The results of the numerical solution of Eqs. (8) are shown in Fig. 2. It is seen that fluctuations do give rise to the re-entrant square-to-rhombus transition in high fields, in a qualitative agreement with SANS data of Fig. 1. In fact, fluctuations change radically the VL phase diagram in high fields, while weakly affecting the low-field branch of \( H_{\parallel} \). The difference between \( H_{\parallel}(T) \) and \( H_{\parallel}(T) \) is significant (except the low-\( T \) clean limit) which justifies the use of the London model. As the ratio \( \rho_0/\zeta_0 \) decreases (e.g., due to nonmagnetic impurities), the region of the square VL on the \( H - T \) diagram shrinks. The raise of the lower branch of \( H_{\parallel}(T) \) has been seen on \( \text{Lu}(\text{Co}_{\alpha}\text{Ni}_{1-\alpha})_2\text{B}_2\text{C} \), for which the mean-free path \( \ell \) was suppressed by Co doping.

It is worth noting that although the calculated curves \( H_{\parallel}(T, \ell) \) reproduce correctly qualitative features of the SANS data of Fig. 1, actual position of the upper branch is sensitive not only to the accuracy with which we know the elastic moduli and the parameters for their evaluation, but also to the precise value of the empirical cutoff constant \( C \), see Eq. (8). The information on the actual position of the upper branch of \( H_{\parallel}(T, \ell) \) is still scarce, and we hope to refine our approximations when the data are available.

Now we comment briefly on the possible effect of the VL transition on the flux pinning. Since the instability of the square VL at \( H_{\parallel} \) is not accompanied by divergence of \( u^2 \), the critical current density \( J_c \), evaluated within the collective pinning theory, should not be sensitive to the VL transition. Indeed, the correlation function of vortex displacements \( \langle u(r)u(r') \rangle \) can be evaluated with the help of Eq. (8) in which \( T \) is replaced by \( \gamma_p \exp(k(r-r')) \), where \( \gamma_p \) is the pinning parameter. The \( H_{\parallel} \), the squish modulus vanishes, but \( \langle u(r)u(r') \rangle \) remains of the same order as for a triangular London VL, to the accuracy of the weak logarithmic factor \( \eta \sim \ln(\xi/\rho b^{1/4}) \sim 1 \). Thus, contrary to the claim of Ref. [14], neither the pinning correlation length nor \( J_c \) are significantly affected by the squish softening near \( H_{\parallel} \).

The two-valued \( H_{\parallel}(T) \) and the re-appearance of the triangular VL at \( H \to H_{\parallel} \) are generic features which are not limited to nonmagnetic borocarbides. The low-\( T \) SANS experiments on antiferromagnetic \( \text{TmNi}_2\text{B}_2\text{C} \) have revealed the triangular VL near \( H_{\parallel} \), which evolves into a square as the field decreases. At this stage the effect of antiferromagnetic ordering upon VLs is unclear, but fluctuations could certainly contribute to the re-entrant VL transition in \( \text{TmNi}_2\text{B}_2\text{C} \) as they do in \( \text{LuNi}_2\text{B}_2\text{C} \). Similar behavior was seen in \( \text{YNi}_2\text{B}_2\text{C} \). Another candidate for studying effects of vortex fluctuation is \( \text{V}_3\text{Si} \), in which the rhombic VL was observed at \( T < 5^\circ \text{K} \) and \( H = 10 \text{ kOe} \) \( (H_{\parallel} \approx 15 \text{ kOe}) \); as \( T \) increases at the fixed field, the rhombic VL evolves toward the hexagonal one as \( T \to T_{\text{c}2}(H) \).

In conclusion, we present a model of the structural VL transition at \( H_{\parallel}(T) \) affected by thermal fluctuations of vortices. We show that the curves \( H_{\parallel}(T) \) and \( H_{\parallel}(T) \) do not cross, instead \( H_{\parallel}(T) \) becomes two-valued. The upper branch of \( H_{\parallel}(T) \) corresponds to a re-entrant transition of the rhombic VL, in accordance with recent SANS observations on \( \text{LuNi}_2\text{B}_2\text{C} \).

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![FIG. 1. The transition line \( H_0(T) \) (circles) in LuNi$_2$B$_2$C observed by SANS [17]. The inset shows \( H_0(T) \) (dashed line) predicted by the extended GL theory [6] without vortex fluctuations. The solid lines shows \( H_{c2}(T) \).](image)

![FIG. 2. The transition lines \( H_0(T) \) obtained by numerically solving Eq. (1) for \( \chi_0 = 0.0064 \), \( C = 1 \), and a few ratios of \( \rho/\xi_0 \). The dashed line is \( H_{c2}(T) \).](image)