Correlation Lengths in the Vortex Line Liquid of a High-T_c Superconductor

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We use the three dimensional uniformly frustrated *XY* model as a model for a high temperature superconductor in an applied magnetic field and explicitly measure the longitudinal correlation length ξ_z in the vortex line liquid phase. We determine the scaling of ξ_z with magnetic field and system anisotropy close to the vortex lattice melting transition. We apply our results to determine the extent of longitudinal correlations in YBCO just above melting. [S0031-9007(99)08645-7]

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It is now generally accepted that thermal fluctuations in the high T_c superconductors lead, for a clean sample in the mixed state, to a first order melting of the vortex line lattice into a vortex line liquid. The properties of this vortex line liquid have been the subject of considerable investigation. An early theory by Feigel'man and coworkers [1] proposed that longitudinal (parallel to the applied field H) superconducting coherence could still persist above melting. Flux transformer experiments in heavily *twinned* YBCO single crystals [2] suggested support for this conclusion, as did early numerical simulations [3,4] of the frustrated three dimensional (3D) *XY* model. However, more recent experiments on *untwinned* YBCO single crystals by López *et al.* [5] found longitudinal coherence to vanish simultaneously with melting, as have recent, more extensive, *XY* simulations by Hu *et al.* and by Nguyen and Sudbø [6]. However, it remains an important open question just how large the finite longitudinal correlations can become just above melting. Simulations by Nordborg and Blatter [7] within the "two dimensional (2D) boson" approximation, as well as general theoretical considerations [8], predict a correlation length $\xi_z \sim \gamma^{-1} a_{\rm v}$, where $\gamma \equiv \lambda_z/\lambda_\perp$ is the anisotropy ratio and $a_{\rm v} = \sqrt{\phi_0/B}$ is the average spacing between vortex lines. However, analyses of experiments on untwinned single crystal YBCO by Righi *et al.* [9] and by Moore [10] have suggested that longitudinal correlations may be of the surprisingly larger micron scale.

To investigate this issue, we carry out extensive new simulations of the frustrated 3D *XY* model for different values of applied flux density f and anisotropy η, explicitly measuring the longitudinal correlation length ξ_z as determined by several different criteria. We find a good scaling of ξ_z with f and η in the continuum limit, allowing us to estimate $\xi_z(T_c)$ in real YBCO single crystal samples. We find that longitudinal correlations at melting are enhanced with respect to the 2D boson approximation, but not dramatically so. We also address several additional questions. We show, contrary to recent claims [11], that there is only a single transition even in the isotropic model. In the very anisotropic limit $\xi_z(T_c) < d$, where a crossover to 2D behavior has been predicted [8,12], we find no qualitative differences from the less anisotropic cases. We find that thermally excited vortex loops, which become important at low magnetic fields, can be described by an effective renormalization of the interaction between field induced vortex lines, and we find no evidence for a recently proposed transition within the vortex line liquid phase [13,14].

Our model is the uniformly frustrated 3D *XY* model [15], given by the Hamiltonian

$$\mathcal{H}[\{\theta_i\}] = -\sum_{i,\hat\mu} J_\mu \cos(\theta_i - \theta_{i+\hat\mu} - A_{i\mu}), \quad (1)$$

where the sum is over the sites i of a cubic grid of points with unit basis vectors $\hat\mu = \hat x, \hat y, \hat z$. θ_i is the phase angle of the superconducting wave function on site i, and $A_{i\mu} = (2\pi/\phi_0)\int_i^{i+\hat\mu} \mathbf{A}\cdot d\mathbf{l}$ is the integral of the magnetic vector potential on the specified bond. The unit of the grid spacing along $\hat z$ is taken as d, the spacing between the weakly coupled CuO planes; the unit of the grid spacing in the xy plane is taken as $\xi_{\perp 0}$, the bare vortex core size in the plane. The Hamiltonian (1) results from making the London approximation to the discretized Ginzburg-Landau energy, and assuming $\lambda/a_{\rm v} \longrightarrow \infty$ so that the internal magnetic field $\mathbf{B}$ can be taken as frozen and equal to the uniform applied field $\mathbf{H}$. For a uniaxial anisotropic system with weak direction along $\hat z$, the couplings are $J_{x,y} \equiv J_\perp = \phi_0^2 d/(16\pi^3\lambda_\perp^2)$ and $J_z = \phi_0^2\xi_{\perp 0}^2/(16\pi^3\lambda_z^2 d)$, where $\lambda_\perp$ and λ_z are the penetration lengths in the respective directions. The anisotropy is given by the parameter

$$\eta \equiv \sqrt{\frac{J_\perp}{J_z}} = \frac{\lambda_z}{\lambda_\perp}\frac{d}{\xi_{\perp 0}} \equiv \gamma\frac{d}{\xi_{\perp 0}}, \quad (2)$$

and the magnetic field is taken uniform along $\hat z$, with a density of flux quanta per plaquette of the grid,

$$f \equiv B\xi_{\perp 0}^2/\phi_0 = (\xi_{\perp 0}/a_{\rm v})^2. \quad (3)$$

f and η are the two dimensionless parameters of our model. A more complete derivation of Eq. (1), and justification for its use in modeling high T_c materials, is given in Ref. [4]. Its advantage over the "2D boson" approximation is in its more realistic vortex line interaction, and in that it allows for the production of thermally activated vortex ring excitations, which may be important at small f.

To determine the relevant transitions in the model, we simulate Eq. (1) with periodic boundary conditions [16], measuring the standard quantities [17]: (i) the helicity moduli parallel and perpendicular to the field, Υ_z and $\Upsilon_\perp$, which measure phase coherence, and (ii) $\Delta S(\mathbf{K}) = S(\mathbf{K}) - S(R_x[\mathbf{K}])$, where $S(\mathbf{k}_\perp)$ is the average intraplanar vortex structure function, $\mathbf{K}$ is a reciprocal lattice vector of the ordered vortex lattice, and R_x reflects $\mathbf{K}$ through the x axis; the difference is used so that ΔS vanishes in the liquid, and we average ΔS over the three smallest nonzero values of $\mathbf{K}$. Our simulations at temperatures near the transition, for a lattice of size $L_\perp \times L_\perp \times L_z$, consist typically of $L_\perp^2 L_z$ Monte Carlo passes through the entire lattice for equilibration [18], followed by 2×10^6–10^7 passes for computing averages.

An example of our results is shown in Fig. 1 below for the case of isotropic couplings $\eta = 1$, and $f = 1/20$, for $L_\perp = 40$ and several different sizes L_z. If we denote the loss of longitudinal coherence, where Υ_z vanishes, as T_c, and the melting of the vortex lattice, where ΔS vanishes, as T_m, then only for the largest L_z do we clearly observe a single transition with $T_m = T_c$ [19]. The strongest finite size effect is the *increase* in T_m as L_z increases. Our results explain recent simulations by Ryu and Stroud [11] which, using smaller systems, continued to suggest $T_m < T_c$ for the isotropic model. Note that $\Upsilon_\perp$ vanishes well below T_c, indicating that the vortex lattice has depinned from our numerical grid well below its melting.

We next measure the longitudinal correlation lengths in the vortex line liquid, $T_c < T$, as determined three different ways. The phase angle correlation length ξ_z and the vortex correlation length ξ_{vz} are defined by the correlation functions,

$$C(z) \equiv \langle e^{i[\theta(\mathbf{r}_\perp, z) - \theta(\mathbf{r}_\perp, 0)]} \rangle \sim e^{-z/\xi_z}, \qquad T_c < T, \quad (4)$$

$$C_v(z) \equiv \langle n_z(\mathbf{r}_\perp, z) n_z(\mathbf{r}_\perp, 0) \rangle \sim e^{-z/\xi_{vz}}, \qquad T_c < T. \quad (5)$$

Here $n_z(\mathbf{r}_\perp, z) = \frac{1}{2\pi}[\mathbf{D} \times \mathbf{D}\theta] \cdot \hat{z}$ is the vorticity in the xy plane at transverse position $\mathbf{r}_\perp$ and height z ($\mathbf{D}$ is the lattice difference operator). We work in a gauge for which $A_{iz} = 0$. Our third length is determined by considering the wave vector dependent helicity modulus $\Upsilon_z(\mathbf{k}_\perp)$, which gives the linear response in supercurrent to a perturbation in vector potential $A_z(\mathbf{k}_\perp)$ [20]. In $D = 3$, dimensional analysis gives $\Upsilon_z \sim 1/\text{length}$. In the vortex liquid, provided one is not near any critical point where anomalous dimensions might come into play [21], $\Upsilon_z(\mathbf{k}_\perp)$ must vanish as $k_\perp^2$ as $k_\perp \longrightarrow 0$. We therefore define the helicity correlation length $\xi_{\Upsilon z}$ by

$$\Upsilon_z(\mathbf{k}_\perp) \equiv c\,\xi_{\Upsilon_z} k_\perp^2, \qquad T_c < T, \quad (6)$$

where c is a constant numerical factor, which we fix in an *ad hoc* manner by requiring $\xi_{\Upsilon z} = \xi_z$ at $T = 1.2$.

For each case we have considered, we first carefully choose L_z sufficiently large so as to observe a single sharp first order melting transition; however, L_z must not be *too* large, in order that we are still able to cool into the vortex lattice state without getting trapped in a supercooled liquid. For such a value of L_z, we carefully monitor the time sequence of ΔS and determine T_c as the temperature at which the system seems to be switching equally between vortex lattice and vortex liquid states. To accurately measure correlation lengths, we then repeat the simulations with a larger value of $L_z \gg \xi_z(T_c)$, cooling down to the predetermined T_c.

In Fig. 2 we show results for ξ_z, ξ_{vz}, and $\xi_{\Upsilon z}$ vs T, for the case of $f = 1/20$, $\eta^2 = 9$, with $L_\perp = 40$ and $L_z = 128$ (for $T \geq 0.8$, $L_z = 64$). We also show the specific heat C, as computed from energy fluctuations. The peak in C at "T_{c2}" is identified as the crossover where, upon cooling, local superconducting order first develops [4].

We see that all three lengths increase similarly as one cools towards T_c. No noticeable feature is seen near T_{c2}. ξ_z is slightly larger than ξ_{vz} by a factor of about 1.3. The numerical factor of Eq. (6) is found to be $c = 74$. In determining ξ_z and ξ_{vz} from Eqs. (4) and (5), we fit our data self-consistently within the range $\xi_z < z < L_z/3$, averaging over the position $\mathbf{r}_\perp$. In determining $\xi_{\Upsilon z}$, we fit Eq. (6) to the two smallest nonzero values of $k_\perp$, since we found that $\Upsilon_z(\mathbf{k}_\perp)$ quickly saturated to a constant as $k_\perp$ increased. This unfortunately limits the accuracy with which we can determine $\xi_{\Upsilon z}$. Some examples of our fits for ξ_z and $\xi_{\Upsilon z}$ are shown in Fig. 3 below. In the remainder of this work we now focus on the phase correlation length ξ_z.

In Fig. 4 we show our results for ξ_z vs T, for several different values of the parameters f and η.

We can now argue as follows for the dependence of ξ_z on f and η. For small values of f, such that $\xi_{\perp 0} \ll a_v$, we expect that ξ_z should be independent of the vortex core size $\xi_{\perp 0}$. From Eqs. (2) and (3) we see that the only combination of f and η that is independent of $\xi_{\perp 0}$ is $f\eta^2$. Furthermore, for large ξ_z we expect our discretizing grid to become a reasonable approximation of the continuum and

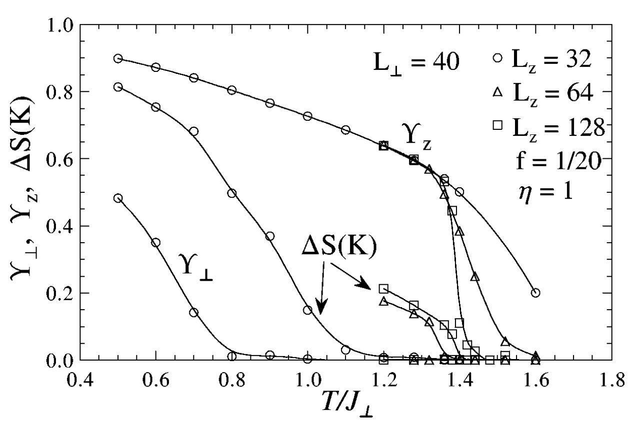

FIG. 1. Helicity moduli $\Upsilon_\perp, \Upsilon_z$, and vortex structure order parameter $\Delta S(\mathbf{K})$ vs T, for $f = 1/20$ and isotropic couplings $\eta = 1$, at system sizes $L_\perp = 40$ and $L_z = 32$, 64, and 128. Solid lines are guides to the eye.

so ξ_z should be independent of the layer spacing d. We therefore expect that the dimensionless ξ_z/d should scale as $1/d$, and so we conclude $\xi_z/d \sim 1/\sqrt{f\eta^2}$. In Fig. 5 below we replot the results of Fig. 4 as $(\xi_z/d)\sqrt{f\eta^2}$ vs T/T_c. We see that as $T \longrightarrow T_c$, most of the data collapse to a single curve. Deviations from this curve represent situations when either ξ_z/d is small $\sim O(1)$, or when T is sufficiently large (approaching T_{c2}) that thermally excited vortex rings start to dominate the total vorticity of the system. In the first case, the discreteness of our grid spacing d clearly becomes an important length scale. In the second case, as the density of thermal rings is determined by the vortex core energy, and hence by the core sizes d and $\xi_{\perp 0}$, again the discreteness of our grid becomes evident. Such deviations thus occur for all cases at sufficiently high T, and also for the case $f = 1/32$, $\eta^2 = 1250$ at all T. This latter case was specifically chosen so that, according to continuum expressions, one would expect $\xi_z(T_c) < d$ and so to be in the so-called "2D" limit of very weakly coupled layers [8,12]. We see that for this case $\xi_z(T_c)/d$ lies below the other data, indicating an even smaller correlation length than one would expect in a continuum. However, we otherwise found no anomalous behavior for this case: there remained only a single transition where longitudinal coherence and vortex lattice order vanished simultaneously.

Except for the "2D" case discussed above, our other data, when appropriately scaled as in Fig. 5, all coincide at T_c. We therefore conclude that, for these cases, our model is well approximating continuum behavior. From the specific numerical value of $(\xi_z/d)\sqrt{f\eta^2}$ at T_c in Fig. 5 we can therefore conclude that in a uniaxial anisotropic superconductor in the "3D" continuum limit,

$$\xi_z(T_c) \simeq 5.5d/\sqrt{f\eta^2} = 5.5\gamma^{-1}a_{\rm v}\,, \qquad (7)$$

where the second equality follows from Eqs. (2) and (3), with $\gamma \equiv \lambda_z/\lambda_\perp$ the anisotropy, and $a_{\rm v}$ the average spacing between vortex lines. Applying this result to YBCO, for which $\gamma \sim 7$, we conclude that $\xi_z(T_c) \simeq 0.86a_{\rm v}$, or $\xi_z \simeq 0.023\mu$ for a field of $B \simeq H = 4$T.

Our result above may be compared with that of recent "2D boson" simulations of Nordborg and Blatter [7], which yielded $\xi_{{\rm v}z}(T_c) = 1.7\gamma^{-1}a_{\rm v}$. If we take from Fig. 2 that $\xi_z(T_c) \simeq 1.3\xi_{{\rm v}z}(T_c)$, then the more realistic vortex line interaction of the *XY* model gives roughly a 2.5 fold increase in $\xi_z(T_c)$ over the boson model. This remains, however, well below the micron scale.

Except for the case $f = 1/100$, our numerical results are all in the limit of sufficiently large f, such that $T_c(f,\eta)$ lies well below the zero field critical point $T_c(0,\eta)$. For these cases, therefore, thermally excited vortex rings are *not* playing any significant role at our melting transitions. One way to see this is to note that for these cases, the melting temperatures $T_c(f,\eta)$ obey quite well the expectation of the Lindemann criterion (which ignores thermal rings), $T_c/J_\perp \propto 1/\sqrt{f\eta^2}$ [4]. To see this, note our result above that $\xi_z(T_c)/d \propto 1/\sqrt{f\eta^2}$, and hence, if the Lindemann criterion holds, we expect $[\xi_z(T_c)/d]/[T_c/J_\perp]$ to be a constant. In Fig. 4 we see that the loci of points $([\xi_z(T_c)/d],[T_c/J_\perp])$ do indeed lie on quite close to a straight line intersecting the origin.

The case $f = 1/100$, however, clearly lies off this line. This is as expected: as f decreases and $T_c(f,\eta)$ increases, one eventually enters the critical region of the $f = 0$ transition, where thermally excited rings play a significant role in renormalizing the effective interactions between the magnetic field induced vortex lines, and suppress the melting transition below the value predicted by the "bare" Lindemann criterion, so that $\lim_{f\longrightarrow 0} T_c(f,\eta) = T_c(0,\eta)$. In this case, our argument that $\xi_z(T_c)$ should be independent of $\xi_{\perp 0}$ becomes less obvious. Nevertheless, we see in Fig. 5 that the data for $f = 1/100$ agree quite well with our scaling assumption in the near vicinity of T_c. We therefore conclude that the main effect of the thermally excited rings at melting is indeed adequately described by a renormalization of vortex line couplings [22], and so our result of Eq. (7) will continue to hold in the low field region, although with a possible renormalization of the anisotropy parameter γ.

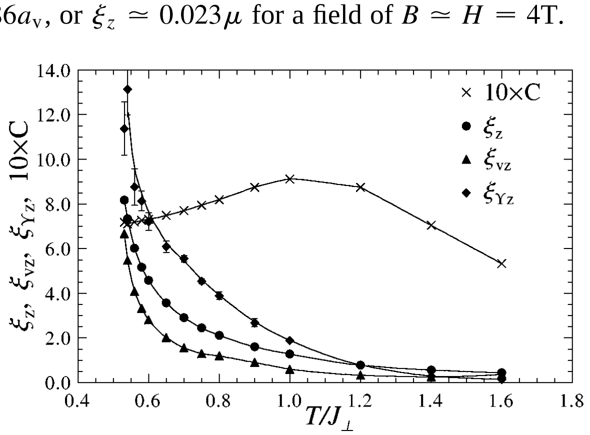

FIG. 2. Phase, vortex, and helicity correlation lengths, ξ_z, $\xi_{{\rm v}z}$, and $\xi_{\Upsilon z}$ vs T for $f = 1/20$ and $\eta^2 = 9$, for system size $L_\perp = 40$ and $L_z = 128$. Also shown is the specific heat C. Solid lines are guides to the eye.

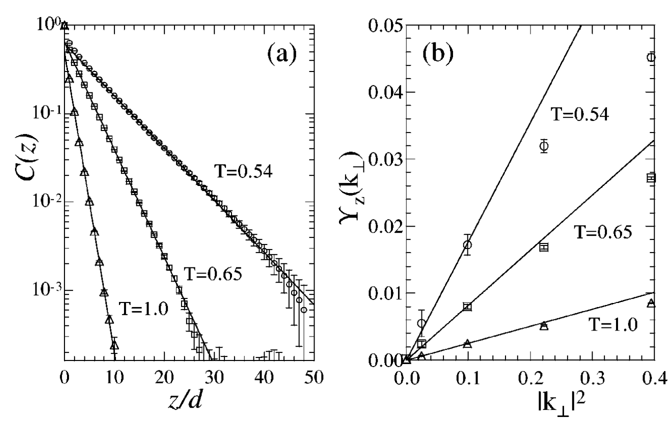

FIG. 3. (a) Phase correlation $C(z)$ vs z, and (b) helicity $\Upsilon_z(\mathbf{k}_\perp)$ vs $k_\perp$, for several different values of T for the parameters of Fig. 2. The solid lines are fits to Eqs. (4) and (6) that determine ξ_z and $\xi_{\Upsilon z}$.

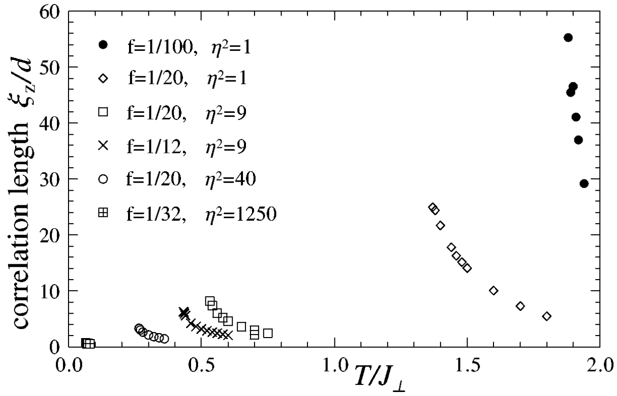

FIG. 4. Phase correlation length ξ_z vs T for parameter values $f = 1/20$ and $\eta^2 = 1$, 9, and 40 (system sizes are $L_\perp = 40$ and $L_z = 192$, 128, and 32 respectively); $f = 1/12$ and $\eta^2 = 9$ (system size is $L_\perp = 24$ and $L_z = 64$); $f = 1/32$ and $\eta^2 = 1250$ (system size is $L_\perp = 64$ and $L_z = 8$); and $f = 1/100$ and $\eta^2 = 1$ (system size is $L_\perp = 100$ and $L_z = 256$).

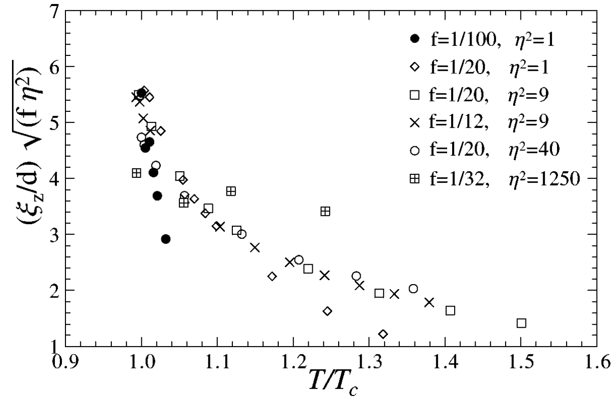

FIG. 5. Data of Fig. 4 replotted as $(\xi_z/d)\sqrt{f\eta^2}$ vs T/T_c.

Recently, Tešanović [13] has argued that there may still be a singular vortex ring blowup transition at low fields, within the normal vortex line liquid. Recent *XY* simulations by Nguyen and Sudbø [14] have claimed to identify this transition in terms of a sharp percolation transition of transverse vortex paths, which takes place in the vicinity of the peak in the specific heat. They find that, within the *XY* model, this percolation transition is more clearly distinct from the melting transition at *larger* rather than *smaller* fields. One of Tešanović's predictions is that the length $\xi_{\Upsilon z}$ will have a discontinuous decrease at this transition. This prediction has been one of our motivations in computing $\xi_{\Upsilon z}$. In Fig. 2 we find no clear evidence for such behavior in $\xi_{\Upsilon z}$. It therefore remains unclear, if such a percolation or ring blowup transition does exists, whether it has any noticeable effect on thermodynamically measurable quantities.

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[17] See Eqs. (10) and (11) of Ref. [4].
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