Structure of a dense vortex-line liquid in a model high-T_c superconductor

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We study the properties of a vortex-line liquid, within a uniformly frustrated three-dimensional XY model, as a model for a type-II high-T_c superconductor. The vortex structure function $S(\mathbf{q}_\perp, q_z)$ is computed with Monte Carlo simulations, and our results compared with hydrodynamic and two-dimensional boson approximations. Properties of the elastic moduli are discussed.

Much recent research on the type-II high-T_c superconductors has concerned fluctuations of the vortex lines in the mixed phase. As temperature T is lowered below the onset of sizable reversible magnetization, $T_{c2}(H)$, a vortex-line liquid phase[1] is believed to exist, until the "irreversibility line" is reached at lower T where the vortex-line liquid freezes[2] (into either a lattice,[3,4] or pinned vortex-line glass[5]). Several theoretical works have sought to describe behavior in this line liquid phase.[3,6–13] A particular quantity of interest is the vortex structure function[3,7,9] $S(\mathbf{k})$ which measures correlations between the vortices in the planes perpendicular to the applied magnetic field. From $S(\mathbf{k})$ one may extract correlation lengths, and infer properties of the effective elastic moduli of the fluctuating line liquid. In this paper we use Monte Carlo simulations to calculate $S(\mathbf{k})$ within a simplified model of a high-T_c superconductor, the uniformly frustrated three-dimensional XY model. This model has been previously introduced by us[13] to investigate vortex-line lattice melting, and vortex-line cutting, and applies in the high field, dense line limit, where the magnetic penetration length $\lambda \gg a_v$, the average spacing between lines. We compare our results against the hydrodynamic[7,9] and two-dimensional boson approximations.[7]

Our model is given by the Hamiltonian

$$\mathcal{H} = J_0 \sum_{\langle ij\rangle} V(\theta_i - \theta_j - A_{ij}), \tag{1}$$

where θ_i is the phase of the superconducting wave function at site i, $A_{ij} \equiv (2e/\hbar c)\int_i^j \mathbf{A}\cdot d\mathbf{l}$ is the integral of the vector potential from site i to site j, and the sum is over nearest-neighbor sites of an $L_\perp \times L_\perp \times L_z$ cubic lattice. We assume a uniform magnetic induction $\mathbf{B} = \nabla \times \mathbf{A}$ in the $\hat{\mathbf{z}}$ direction, which induces an average density of $f = Ba^2/\Phi_0$ vortex lines in the ground state (a is the lattice constant, Φ_0 is the flux quantum). We use the Villain interaction[14]

$$V(\alpha) \equiv -(T/J_0)\ln\left(\sum_{m=-\infty}^{\infty} \exp[-\tfrac{1}{2}J_0(\alpha - 2\pi m)^2/T]\right) \tag{2}$$

as opposed to the cosine interaction of our previous study, in order to eliminate the coupling between spin wave and vortex excitations of the Hamiltonian (1).

A standard duality transformation[15] gives the interaction between the vortex lines of (1) as

$$\mathcal{H}_v = 2\pi^2 J_0 \sum_{i,j}\sum_{\mu} n_\mu(i) n_\mu(j) G(\mathbf{r}_i - \mathbf{r}_j), \tag{3}$$

where $n_\mu(i)$ is the integer vorticity of the face with normal $\hat{\boldsymbol{\mu}} = \hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}$ of the unit cell centered at the dual lattice site i. G is the lattice Green's function which solves $D_{ij}G(\mathbf{r}_j - \mathbf{r}_k) = -\delta_{i,k}$, where D_{ij} is the lattice Laplacian. $G(\mathbf{r}) \simeq 1/(4\pi r)$ for $r \gg a$. Taking Fourier transforms, $n_\mu(\mathbf{k}) \equiv \sum_i n_\mu(i)\exp(i\mathbf{k}\cdot\mathbf{r}_i)$, we have

$$\mathcal{H}_v = \frac{2\pi^2 J_0}{N}\sum_{k,\mu} n_\mu(\mathbf{k}) n_\mu(-\mathbf{k}) G_k, \tag{4}$$

where $N = L_\perp^2 L_z$, and

$$\begin{aligned} G_k &= 1/K^2 = 1/(K_z^2 + K_\perp^2),\\ K_z^2 &\equiv 2 - 2\cos k_z a,\\ K_\perp^2 &\equiv 4 - 2\cos k_x a - 2\cos k_y a. \end{aligned} \tag{5}$$

Note $K^2 \simeq (ka)^2$ for small ka, however they are different at large ka due to the discreteness of the lattice.

This model describes a lattice version of an isotropic type-II superconductor where $J_0 \equiv \Phi_0^2/(16\pi^3\lambda^2)$. The coherence length is $\xi_0 \sim a$. Since the interaction between vortex lines is $G_k = 1/K^2$ instead of the London[16] $1/(K^2 + \lambda^{-2})$, our model will only be correct for describing fluctuations of a superconductor on scales $k > \lambda^{-1}$. However for the high-T_c materials, λ/ξ_0 is generally large, so that for a wide range of applied magnetic field $H_{c1} < H \le H_{c2}$, $\lambda \gg a_v$, the average vortex spacing. For such H, our model will apply in the wide range of interest $\lambda^{-1} < k \lesssim a_v^{-1}$.

Following the works of Marchetti[9] and Nelson and LeDoussal[7] on continuum vortex lines, it is straightforward to derive the hydrodynamic limit of $S(\mathbf{k})$ for our lattice model. Coarse-grain averaging the microscopic (4) gives a free energy on hydrodynamic scales $k \ll a_v^{-1}$,

$$F = \frac{1}{2Nf^2}\sum_k \left(c_{44}(\mathbf{k})\sum_{\mu_\perp = x,y}[\delta n_{\mu_\perp}(\mathbf{k})\delta n_{\mu_\perp}(-\mathbf{k})] + c_l(\mathbf{k})\delta n_z(\mathbf{k})\delta n_z(-\mathbf{k})\right), \tag{6}$$

where the $\delta n_\mu(\mathbf{k})$ give the deviation from the ground state and are now viewed as independent continuous variables. c_{44} and c_l are the tilt and bulk moduli on the lattice with

$$c_l(\mathbf{k}) = 4\pi^2 f^2 J_R G_k, \quad c_{44}(\mathbf{k}) = c_l(\mathbf{k}) + f\epsilon_1(k_z). \tag{7}$$

We write J_R instead of J_0 to allow for possible renormalization of the coupling constant in the coarse-graining procedure. ϵ_1 is the single-vortex-line tension, which may depend[16,17] on k_z due to the interaction (3) between the different segments of the single line. The difference $c_{44} - c_l$ just gives the additional energy needed to create the elongation of the vortex lines described by the transverse components of the fluctuation.[9] Using $J_R = \Phi_0^2/16\pi^3\lambda_R^2$, (7) are just the usual continuum moduli,[16] in the limit $k \gg \lambda^{-1}$. Similar results have been obtained by Sudbø and Brandt,[17] expanding about the elastic limit of the vortex-line lattice in a continuum.

Using (6) to average over $\delta n_\mu(\mathbf{k})$ subject to the constraint that vortex lines must be continuous, $\sum_\mu n_\mu(\mathbf{k})[1 - \exp(ik_\mu)] = 0$, one finds for the structure function

$$\begin{aligned} S(\mathbf{k}) &\equiv \frac{1}{N}\langle n_z(\mathbf{k}) n_z(-\mathbf{k})\rangle \\ &= \frac{Tf^2K_\perp^2}{c_l(\mathbf{k})K_\perp^2 + c_{44}(\mathbf{k})K_z^2} \\ &= \frac{TK_\perp^2}{4\pi^2 J_R + [\epsilon_1(k_z)/f]K_z^2}. \end{aligned} \tag{8}$$

Defining the Fourier transform, $S(\mathbf{k}_\perp, z) \equiv (1/L_z)\sum_{k_z} S(\mathbf{k}_\perp, k_z)\exp(-ik_z z)$, if the pole of $S(\mathbf{k}_\perp, k_z)$ is at small enough k so that the hydrodynamic result (8) is valid, *and* $\epsilon_1(k_z) \simeq \epsilon_1(0)$, we have

$$S(\mathbf{k}_\perp, z) = S(\mathbf{k}_\perp, z=0)e^{-z/\xi(\mathbf{k}_\perp)}, \tag{9}$$

where the decay length satisfies

$$\begin{aligned} 1/\xi(\mathbf{k}_\perp) &\simeq \sinh[1/\xi(\mathbf{k}_\perp)] \\ &= \frac{fTK_\perp^2}{2\epsilon_1(0)S(\mathbf{k}_\perp, z=0)}. \end{aligned} \tag{10}$$

As noted by Nelson and LeDoussal,[7] this result has exactly the same form as Feynman's approximation[18] for the energy spectrum of a two-dimensional superfluid Bose gas, with the identifications: $\hat{z}$ ≡ time axis, $\epsilon_1(0)$ ≡ the boson mass, $T \equiv \hbar$, $S(\mathbf{k}_\perp, z=0)/f$ ≡ the two-dimensional static form factor for neutron scattering off the boson fluid, $1/\xi(\mathbf{k})$ ≡ the frequency (energy) spectrum of the superfluid excitations. Nelson[3,6,7] has extended this analogy by introducing the "two-dimensional boson approximation," in which the full three-dimensional interaction between all vortex-line segments (3) is replaced by an effective two-dimensional interaction between segments which lie in the same z plane ("equal time boson interaction"), and hence $\epsilon_1(k_z) \to \epsilon_1(0)$, all k_z ("frequency independent boson mass"). The result of a Feynman approximation[7] in this two-dimensional boson system is that (10) should hold at all $\mathbf{k}$, not just in the hydrodynamic limit. This is equivalent to assuming that, at all $\mathbf{k}$, $S(\mathbf{k})$ satisfies the relation[7,19]

$$TK_\perp^2/S(\mathbf{k}_\perp, k_z) = 4\pi J_R(\mathbf{k}_\perp) + [\epsilon_1(0)/f]K_z^2. \tag{11}$$

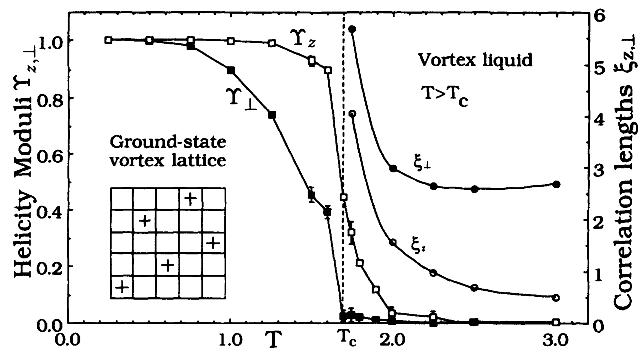

FIG. 1. Helicity moduli $\Upsilon_{z,\perp}$ and correlation lengths $\xi_{z,\perp}$ parallel and perpendicular to the magnetic induction $\mathbf{B}$. $\Upsilon_{z,\perp} \to 0$, $\xi_{z,\perp} \to \infty$ locates the superconducting, vortex lattice melting transition $T_c \simeq 1.7$. The inset shows the positions of the vortex lines in their ground-state lattice, in a plane perpendicular to $\mathbf{B}$.

To investigate these predictions for $S(\mathbf{k})$ we have carried out Metropolis Monte Carlo simulations of the Hamiltonian (1). The results presented below are for an $N = 20^3$ lattice, with periodic boundary conditions in all directions. We consider the case $f = \frac{1}{5}$, giving 80 vortex lines in our system. The unit cell of the ground-state vortex lattice ($a_v = \sqrt{5}$) is shown as the inset to Fig. 1. We use typically 30 000 passes through the lattice to compute averages, after 5 000 passes for equilibration. Henceforth, energy scales will be quoted in units of J_0, and lengths in units of a. A simple algorithm[13] locates the vortex lines in the phase variables θ_i, and allows a direct computation of $S(\mathbf{k}_\perp, z)$ which we Fourier transform to obtain $S(\mathbf{k}_\perp, k_z)$. The allowed wave vectors are given by $k_\mu = 2\pi m_\mu/L_\mu$, $m_\mu = 0, \ldots, L_\mu - 1$. We have considered here only the values of $\mathbf{k}_\perp \equiv (k_x, k_y) = (2\pi m_\perp/L_\perp)(2,1)$, in the direction of the shortest periodicity of the ground-state vortex-line lattice; for $T < T_c$, $S(\mathbf{k}_\perp, z=0)$ has a pth Bragg peak at $|\mathbf{k}_\perp| = 2\pi p/a_v$, or $m_\perp/L_\perp = p/5$ (for $L_\perp = 20$, these occur at $m_\perp = 4, 8$).

In Fig. 1 we show our results for the helicity moduli $\Upsilon_{z,\perp}$ and liquid phase correlation lengths $\xi_{z,\perp}$, parallel and perpendicular to the magnetic field. $\Upsilon_{z,\perp}$ is computed using the standard fluctuation relation.[20] $\xi_z \equiv \xi(k_\perp = 2\pi/a_v)$ is obtained from a fit to Eq. (9) and is just Nelson's "entanglement correlation length."[3,6,7] $\xi_\perp$ is estimated from the width of the peak in $S(\mathbf{k}_\perp, z=0)$. As T increases, $\xi_z \to\sim 1$ the spacing between planes, while $\xi_\perp \to a_v = \sqrt{5}$ the average spacing between vortex lines in the plane. $\Upsilon_{z,\perp} \to 0$ gives $T_c \simeq 1.7$ as the superconducting transition temperature where phase coherence is lost. The divergence of $\xi_{z,\perp}$ at T_c indicates that this is also the vortex-line lattice melting temperature. The increasing ratios $\Upsilon_z/\Upsilon_\perp$ and $\xi_z/\xi_\perp$ as T_c is approached from both below and above, are suggestive of the proposed anisotropic scaling in this system.[3]

In Fig. 2 we show the values of J_R and $\epsilon_1(0)$, resulting

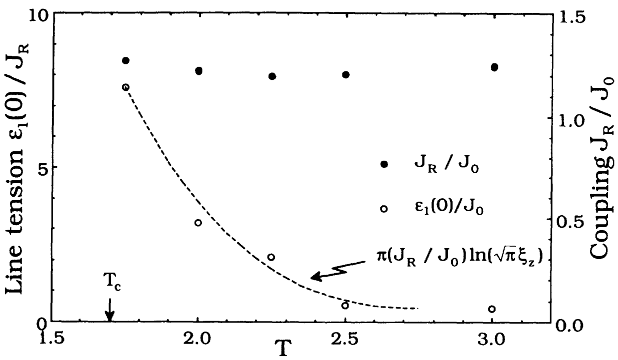

FIG. 2. Hydrodynamic parameters J_R and $\epsilon_1(0)$ from fitting to Eq. (8). The line tension $\epsilon_1(0)$ is in good agreement with the form $\pi J_R \ln(\sqrt{\pi}\xi_z)$, shown as the dashed line. ξ_z is taken from Fig. 1.

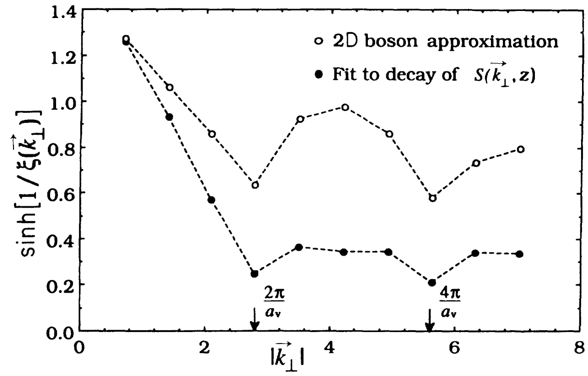

FIG. 4. Decay length $\xi(k_\perp)$ vs $k_\perp$ obtained from fitting data to Eq. (9), compared with the two-dimensional boson approximation Eq. (10). The minima occur at the Bragg peaks of the $T < T_c$ line lattice. Data is for $T = 1.75$.

from a fit to the hydrodynamic form (8), as $k \to 0$. The coupling shows a noticeable renormalization, $J_R \simeq 1.2 J_0$. The line tension $\epsilon_1(0)$ is found to decrease to zero as T increases above T_c. We can understand this behavior as follows. For $\lambda \gg \xi_0$, the line tension of an isolated line, as first given by Abrikosov, is $\epsilon_1(0) = (\Phi_0/4\pi\lambda)^2 \ln(\lambda/\xi_0) = \pi J_0 \ln(\lambda/\xi_0)$. In our lattice model, although the range of the *bare* vortex interaction is $\lambda \to \infty$, the *screened* interaction in the line liquid phase (where $\Upsilon \to 0$) has a finite range $\sim \xi_z$. This suggests that the hydrodynamic $\epsilon_1(0)$ is given by the above Abrikosov result, but with the replacement $\lambda \to \xi_z$ in the logarithm [or equivalently, using the single line tension[16,17] $\epsilon_1(k_z) \simeq \pi J_0 \ln(1/k_z\xi_0)$ evaluated at $k_z \simeq 1/\xi_z$]. Using the same renormalization factor as found for J_0, and approximating ξ_0 by $\pi\xi_0^2 = a^2 \equiv 1$, we plot in Fig. 2 as the dashed line, $\pi J_R \ln(\sqrt{\pi}\xi_z)$, using $\xi_z(T)$ from Fig. 1. Provided ξ_z is not too small (so that the Abrikosov result remains valid), we find good agreement with the hydrodynamic $\epsilon_1(0)$. When $\xi_z \lesssim 1$, $\epsilon_1(0) \sim 0$, and the planes decouple.[19,21]

In Figs. 3(a) and 3(b) we plot the quantity $TK_\perp^2/S(\mathbf{k}_\perp, k_z)$ [see Eq. (11)] versus K_z^2 and $K_\perp^2$, for $T = 1.75$. In 3(a), the curves correspond to different values of $\mathbf{k}_\perp = (2\pi m_\perp/L_\perp)(2,1)$; in 3(b) the curves are for different values of $k_z = 2\pi m_z/L_z$. The nonlinear shape of the curves in Fig. 3(a), disagrees with the simple form (11), and gives an $\epsilon_1(k_z)$ that decreases as k_z increases, in qualitative agreement with predictions for $c_{44} - c_l$ [see Eq. (7)] from continuum elastic theory.[16,17,21] Lines are softer to bending at smaller wavelengths. Furthermore, although the curves in Fig. 3(a) have qualitatively the same shape, the slopes as $k_z \to 0$ increase as $k_\perp$ increases. Thus to put our data in the form (11), it is necessary to let ϵ_1 depend on both k_z *and* $k_\perp$ (or equivalently let J_R depend on k_z).

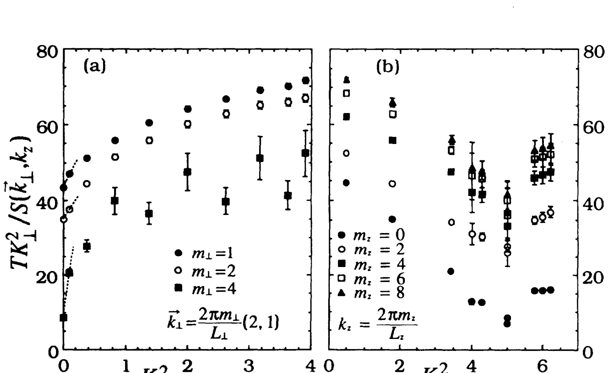

FIG. 3. $TK_\perp^2/S$ vs (a) $K_z^2 = 2 - 2\cos k_z$ and (b) $K_\perp^2 = 4 - 2\cos k_x - 2\cos k_y$, at $T = 1.75$. In (a), the curves are for different $\mathbf{k}_\perp$; $m_\perp = 4$ corresponds to $|\mathbf{k}_\perp| = 2\pi/a_v$. The dashed lines at small K_z indicate the increasing slope for increasing $k_\perp$. In (b) the curves are for different k_z. $|\mathbf{k}_\perp| = 2\pi/a_v$ occurs at $K_\perp^2 = 5$.

While these deviations from the simple form (11) are due in part to the simplicity of the boson model in approximating the three-dimensional interactions of the vortex lines, we point out that the Feynman approximation which gives (11) for the Bose system, is in itself a very simple approximation (it gives a roton minimum twice as large as experiment[18] when applied to three-dimensional superfluid ^{4}He) and that the true two-dimensional boson dynamic structure function may be more complicated than (11).

The $m_z = 0$ curve in Fig. 3(b), gives the $k_\perp$ dependence of the coupling J_R, or via Eq. (7), the bulk modulus, $J_R \propto c_l K^2$. In the hydrodynamic approximation (8) on scales $k_\perp \ll a_v^{-1}$, this is expected to be a constant. In contrast, we see a fairly strong dependence, decreasing as $K_\perp^2$, until a minimum is reached at $k_\perp = 2\pi/a_v$. It would be interesting if such a softening of the macroscopic elastic moduli is also present in the vortex-line lattice phase.

Finally, in Fig. 4 we show the decay length $\xi(\mathbf{k}_\perp)$ versus $k_\perp$, at $T = 1.75$, obtained from fitting our data to Eq. (9). We compare this to the two-dimensional boson approximation Eq. (10). Despite the quantitative inaccuracies of this approximation (as illustrated by Fig. 3) the two curves show the same qualitative behavior, having their minima at $k_\perp = 2\pi p/a_v$, $p = 1, 2$, where the vortex lattice below T_c has its Bragg peaks. That the curves approach a finite value as $k_\perp \to 0$ (i.e., the "boson energy spectrum" is plasmonlike, rather than phononlike) is a consequence of the vortex interaction in our model being long ranged,[19] $G_k = 1/K^2$, rather than the finite ranged $1/(K^2 + \lambda^{-2})$ (had our interaction been the latter, we would expect the curves in Fig. 4 to decrease linearly to zero once $k_\perp$ decreased below λ^{-1}). The two curves agree at small $k_\perp$ because $\epsilon_1(0)$ of Eq. (10) has been obtained from the hydrodynamic fit at small $k_\perp$. At larger $k_\perp$, the boson model gives a factor $\sim 2-3$ too large. Had we instead chosen to apply Eq. (10) using $\epsilon_1(k_z = 0)$ obtained from the slope of the curve in Fig. 3(a) at $k_\perp = 2\pi/a_v$, the two curves in Fig. 4 would agree quite well for $k_\perp \gtrsim 2\pi/a_v$, but disagree at smaller k.

We have checked our results for finite-size effects, by also carrying out simulations on an $N = 10^3$ lattice. We have found no appreciable differences, except very close to T_c. This is not surprising, as over most of the temperature range for which we have analyzed our data, the correlations lengths $\xi_{z,\perp} \lesssim 6$ (see Fig. 1) are significantly smaller than the length $L = 20$ of the system. In particular, we expect our hydrodynamic fits in the vortex-line liquid phase to be valid for $T \geq 1.75$.

To conclude, we have computed the structure function $S(\mathbf{k})$ of a model high-T_c superconductor in the dense line limit, $\lambda \gg a_v$, and extracted from it information about the correlation lengths and elastic moduli in the vortex-line liquid phase. We find that the line tension $\epsilon_1(0)$ decreases in the liquid phase as ξ_z decreases below λ. Our results show the importance of including the full three-dimensional interaction between vortex lines for calculating the correct $\mathbf{k}$ dependence of elastic properties (in particular ϵ_1). Nevertheless we have found that the simplified two-dimensional boson approximation gives qualitatively correct behavior for many interesting features.

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