Superconducting Coherence in a Vortex Line Liquid: Simulations with Finite λ

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We carry out simulations of a lattice London superconductor in a magnetic field **B**, with a finite magnetic penetration length λ. We find that superconducting coherence parallel to **B** persists into the vortex line liquid. We argue that the length scale relevant to this effect is $\Lambda = \phi_0^2/8\pi T_m$.

In high T_c superconductors, thermal fluctuations are believed to melt the ground state vortex line lattice at temperatures well below the mean field H_{c2} line [1,2]. The resulting vortex line liquid has received intense theoretical and experimental study. In particular, recent "flux transformer" experiments [3,4] on YBCO show that superconducting coherence parallel to the applied magnetic field **B** exists over very long length scales well into the vortex liquid.

To investigate the fluctuating vortex line system, numerical simulations have been carried out. These either have involved a simplified model of vortex line interactions [5] or have used the approximation [6–8] that the bare magnetic penetration length $\lambda \longrightarrow \infty$, so that the magnetic field **B** inside the superconductor is uniform. Such $\lambda \longrightarrow \infty$ simulations [8] show a sharp transition within the vortex line liquid, corresponding to the onset of coherence parallel to **B**. While this $\lambda \longrightarrow \infty$ model is suggested by the large values of $\kappa = \lambda/\xi_0$ in the high T_c materials, it may fail close to T_c, where the correlation length may exceed the finite bare λ; thus the finite λ model may display different critical behavior from the $\lambda \longrightarrow \infty$ limit. To investigate this possibility, we present here new simulations of a system of fluctuating vortex lines, in which we include the effect of magnetic screening on the vortex interactions [9], due to a finite λ. We investigate the presence of superconducting coherence within the vortex line liquid, and discuss the length scale relevant for this effect.

Our model is a discretized lattice superconductor in the London limit [10]. For simplicity, we consider isotropic couplings. Following Carneiro, Cavalcanti, and Gartner [7], a duality transformation maps this model onto one of interacting vortex lines, with Hamiltonian

$$\mathcal{H} = 2\pi^2 J_0 \lambda^2 \sum_{i,j} \mathbf{n}(\mathbf{r}_i) \cdot \mathbf{n}(\mathbf{r}_j) G(\mathbf{r}_i - \mathbf{r}_j). \quad (1)$$

Here $n_\alpha(\mathbf{r}_i) (\alpha = x, y, z)$ is the integer vorticity through plaquette α at site $\mathbf{r}_i$ of a cubic mesh of points, and $G(\mathbf{r})$ is the lattice London interaction, with Fourier transform

$$G_q = 1/(1 + \lambda^2 Q^2), \quad Q^2 \equiv \sum_{\mu=x,y,z} [2 - 2\cos q_\mu]. \quad (2)$$

The coupling is $J_0 = \phi_0^2 \xi_0/16\pi^3 \lambda^2$, with ϕ_0 the flux quantum, and ξ_0 the spacing of the discrete mesh, which we identify with the bare coherence length that determines

the size of a vortex core. Henceforth, we measure length in units of ξ_0, and temperature in units of J_0. Periodic boundary conditions in all directions are taken.

To test for superconducting coherence, we consider the helicity modulus $\Upsilon_\mu(q_\nu)$ (where $\mu \neq \nu$), defined as the linear response coefficient giving the supercurrent **j** induced by a transverse perturbation in the vector potential of the externally applied magnetic field, $\delta A_\mu^{\text{ext}}(q_\nu)\hat{\boldsymbol{\mu}}$,

$$j_\mu(q_\nu) = -\Upsilon_\mu(q_\nu)\delta A_\mu^{\text{ext}}(q_\nu). \quad (3)$$

We earlier derived [11] an expression for $\Upsilon_\mu(q_\nu)$ in a continuum London superconductor. The generalization to the lattice superconductor is

$$\Upsilon_\mu(q_\nu) = \frac{[J_0\lambda^2]Q^2}{1 + \lambda^2 Q^2} \left[1 - \frac{4\pi^2 J_0\lambda^2}{VT} \frac{\langle n_\sigma(q_\nu)n_\sigma(-q_\nu)\rangle}{1 + \lambda^2 Q^2} \right], \quad (4)$$

where μ, ν, and σ are a cyclic permutation of x, y, and z, and $Q^2 = 2 - 2\cos q_\nu$ as $q_\mu, q_\sigma = 0$.

In the absence of vortices, $\Upsilon_\mu(q_\nu) = [J_0\lambda^2]Q^2/(1 + \lambda^2 Q^2)$ describes the total screening of the Meissner state. With vortices, an expansion in powers of Q^2,

$$\langle n_\sigma(q_\nu)n_\sigma(q_\nu)\rangle = n_0 + n_1 Q^2 + n_2 Q^4 + \cdots, \quad (5)$$

leads to an expression for $\Upsilon_\mu(q_\nu)$ at small q_ν, in terms of a renormalized coupling $[J\lambda^2]_{\mu R}$ and penetration length $\lambda_{\mu R}$,

$$\Upsilon_\mu(q_\nu) = \frac{[J\lambda^2]_{\mu R}Q^2}{1 + \lambda_{\mu R}^2 Q^2}, \quad (6)$$

with

$$\gamma_\mu \equiv \frac{[J\lambda^2]_{\mu R}}{J_0\lambda^2} = 1 - \frac{4\pi^2 J_0\lambda^2}{VT} n_0, \quad (7)$$

$$\frac{\lambda_{\mu R}^2}{\lambda^2} = 1 + \frac{4\pi^2 J_0}{VT} \frac{n_1 - n_0\lambda^2}{\gamma_\mu}. \quad (8)$$

To see the meaning of γ_μ and $\lambda_{\mu R}$, note that the current $j_\mu(q_\nu)$ produced by $\delta A_\mu^{\text{ext}}(q_\nu)$ induces a magnetic vector potential due to Ampere's law, which in our units is $[J_0\lambda^2]Q^2\delta A_\mu^{\text{ind}}(q_\nu) = j_\mu(q_\nu)$. The change in the total magnetic field due to the external perturbation is therefore given by $\delta A_\mu^{\text{tot}}(q_\nu) = \delta A_\mu^{\text{ind}}(q_\nu) + \delta A_\mu^{\text{ext}}(q_\nu)$, or

$$\delta A_\mu^{\text{tot}}(q_\nu) = \left[(1 - \gamma_\mu) + \gamma_\mu \frac{Q^2}{Q^2 + \lambda_{\mu R}^{-2}} \right]\delta A_\mu^{\text{ext}}(q_\nu). \quad (9)$$

Thus a fraction $1 - \gamma_\mu$ of $\delta A_\mu^{\text{ext}}(q_\nu)$ penetrates into the material; the remaining fraction γ_μ is screened out, on the length scale $\lambda_{\mu R}$. Equivalently, $\lambda_{\mu R}$ is the length on which fluctuations in the magnetic field decay to equilibrium. For a perfect Meissner effect, $\gamma_\mu = 1$ and $\lambda_{\mu R}$ agrees with the usual definition of the London penetration length [12]. We therefore interpret $1/\lambda_{\mu R}^2 \sim \rho_{s\mu}$ as the density of superconducting electron pairs in direction $\hat{\mu}$, even in the more general case of a partial Meissner effect in the mixed state. Although $\Upsilon_\mu(q_\nu)$ will have the same form Eq. (6) in both the superconducting and the normal metal state (with ordinary fluctuation diamagnetism), a transition will be signaled some singularity in γ_μ and $\lambda_{\mu R}$. We focus now on γ_μ.

Consider a uniform applied $\mathbf{H} = H\hat{z}$. $\Upsilon_x(q_y)$ and $\Upsilon_y(q_z)$ then describe the response to external fields $\delta H_z(q_y)$ and $\delta H_x(q_z)$, which represent compression and tilt perturbations of $\mathbf{H}$, respectively. Correspondingly one finds [11]

$$1 - \gamma_x = dB_z/dH_z \quad \text{and} \quad 1 - \gamma_y = dB_x/dH_x, \quad (10)$$

where these susceptibilities are evaluated at the applied field $\mathbf{H}$. Since the high T_c materials display strong fluctuation diamagnetism even in the normal state, it is unclear whether or not $\gamma_{x,y}$ will display a pronounced feature at the superconducting transition.

For behavior along $\hat{z}$, however, parallel to $\mathbf{H}$, the criteria for a superconducting transition is more clearly defined. $\Upsilon_z(q_x)$ describes the response to an external field $\delta H_y(q_x)$, representing a combined shear and tilt perturbation of the uniform applied $H\hat{z}$. In Ref. [11] we showed that for the vortex line lattice one has $\gamma_z = 1$ and a perfect Meissner screening. For a normal vortex line liquid, however, $\gamma_z = 1 - dB_x/dH_x \ll 1$. Thus the transition to the normal state is signaled by a discontinuous jump in γ_z from unity. Expressed in terms of the expansion coefficients of Eq. (5), we have superconducting coherence along the field provided $n_0 = 0$; for the normal state, $n_0 > 0$.

For our Monte Carlo simulation, we start with a fixed density $f = B/\phi_0$ of straight vortex lines parallel to $\hat{z}$, giving the ground state configuration for an internal field $B\hat{z}$. Following Carneiro, Cavalcanti, and Garter [7], we update the system, heating from the ground state, by adding elementary closed vortex rings (a square ring of unit area) with random orientation and position. These excitations are accepted or rejected according to the standard Metropolis algorithm. This provides a complete sampling of phase space for the vortex variables $\mathbf{n}(\mathbf{r}_i)$, subject to the constraints that vorticity is locally conserved, and the average internal field $\mathbf{B} = (\phi_0/V)\sum_i \mathbf{n}(\mathbf{r}_i) = f\phi_0\hat{z}$ is constant.

Our simulations are for the case $f = 1/15$, whose ground state on a cubic mesh is a close approximation to a perfect triangular lattice. We choose $\lambda = 5$, comparable to the vortex line spacing $a_v \equiv 1/\sqrt{f} = 3.87$. We study system sizes $L_\perp = 30$ in the x-y plane, and $L_z = 15$ and

30 parallel to $\mathbf{H}$. Each data point is typically the result of 5000 sweeps to equilibrate, followed by $8-16\,000$ sweeps to compute averages, where each sweep refers to $L_\perp^2 L_z$ attempts to add an elementary vortex ring.

In Fig. 1 we show a sample of our data, plotting $\langle n_y(q_x)n_y(-q_x)\rangle$ vs q_x, for various T, and $L_z = 30$. Fitting by Eq. (5) through $O(Q^4)$ yields the solid curves, and determines the parameters n_0 and n_1. Equation (7) then gives the couplings γ_μ, which we plot vs T in Fig. 2. We see that $\gamma_{x,y}$ decrease towards zero at $T_m \simeq 1.2$, while γ_z decreases at $T_c \simeq 2.0$. We also show our results for $L_z = 15$.

In Fig. 3 we show intensity plots of vortex correlations within the same plane perpendicular to $\mathbf{B}$,

$$S(\mathbf{q}_\perp) = \sum_{z,r_\perp} e^{i\mathbf{q}_\perp \cdot \mathbf{r}_\perp} \langle n_z(\mathbf{r}_\perp, z)n_z(0, z)\rangle, \quad (11)$$

where $\mathbf{q}_\perp = (q_x, q_y)$, for various T, and $L_z = 30$. Below T_m we see sharp Bragg peaks of a vortex line lattice. Above T_m we see behavior characteristic of a liquid. T_m is thus the melting transition. Since the discrete mesh of our simulation acts like a periodic pinning potential for vortices, T_m also coincides with a depinning of the vortex lines. We believe that the drop in $\gamma_{x,y}$ at T_m is more a result of this depinning, rather than a direct result of melting. We expect from Eq. (10) that $\gamma_{x,y} = 1 - dB_x/dH_x$ is finite above T_m, but this value is too small for us to determine accurately.

With respect to coherence along $\mathbf{H}$, we expect a discontinuous jump in γ_z from unity to $1 - dB_x/dH_x \approx 0$ at T_c. The finite width of the decrease observed in our data is a finite size effect; we see that the transition sharpens as L_z increases. We therefore estimate $T_c \simeq 2.0$, well into the vortex line liquid. This is the main result of our simulations.

Recent flux transformer experiments on YBCO [3,4] show that there is a temperature "T_{th}" below which vortex line correlations parallel to $\mathbf{H}$ become comparable to the thickness of the sample. T_{th} is clearly above the "T_{irr}" where resistivity transverse to $\mathbf{H}$ vanishes. Resistivity parallel to $\mathbf{H}$, however, appears [4] to vanish at T_{th}. A similar conclusion concerning vortex line correlations may be inferred from the measurements of Ref. [13],

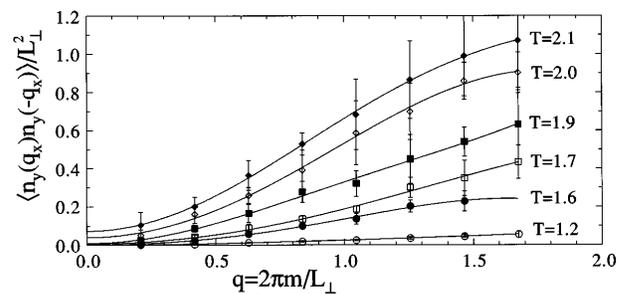FIG. 1. $\langle n_y(q_x)n_y(-q_x)\rangle/L_\perp^2$ vs $q_x = 2\pi m/L_\perp$ (m integer) for various T and $L_\perp = L_z = 30$. Solid lines are a fit by Eq. (5).
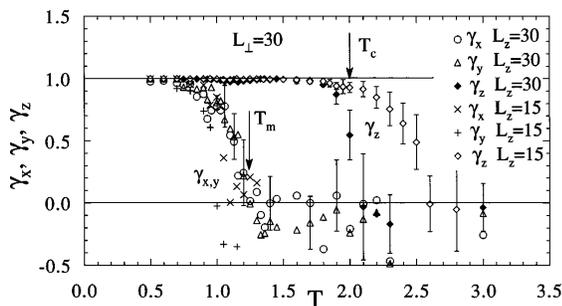
FIG. 2. γ_μ vs T for $L_\perp = 30$ and $L_z = 15, 30$. Sample error bars are shown. $\gamma_{x,y}$ decreases at $T_m \simeq 1.2$; γ_z decreases at $T_c \simeq 2.0$.

where the onset of pinning by twin grain boundaries is shown to occur distinctly above a sharp first order melting transition. If we identify T_{th} with our T_c, and T_{irr} with our T_m, our results are in complete accord with these experimental findings.

We also tried to compute the lengths $\lambda_{\mu R}^2$, using Eq. (8) and our fitted n_0 and n_1. However, the factor $(n_1 - n_0\lambda^2)/\gamma_\mu$ that appears in Eq. (8) is, in the region of the transition, the quotient of two small numbers each with large relative error. We were therefore unable to obtain meaningful results for $\lambda_{\mu R}$.

Although we simulated with $L_z \gg \lambda$, one can still question whether our results represent the true thermodynamic limit. In particular, in Refs. [3,4] it was found that T_{th} decreased towards T_{irr} as sample thickness L_z in-

a) T = 0.50   **b) T = 1.25**

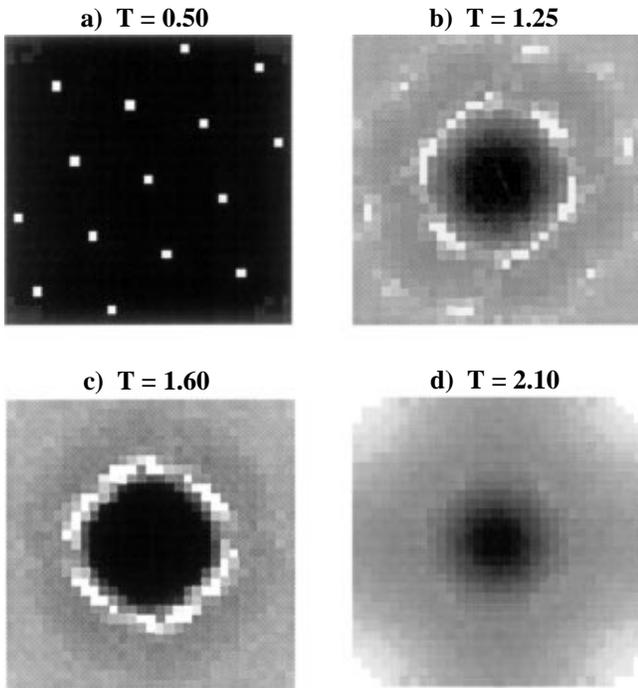**c) T = 1.60**   **d) T = 2.10**

FIG. 3. Intensity plot of $S(\mathbf{q}_\perp)$ for several T and $L_\perp = L_z = 30$. (a) $T = 0.50 < T_m$ shows a lattice of Bragg peaks; (b) $T = 1.25 \approx T_m$; (c) $T_m < T = 1.60 < T_c$ in the vortex line liquid; and (d) $T = 2.10 > T_c$.

creased. This is also consistent with our results for γ_z in Fig. 2, where there is some suggestion that, in addition to a sharpening of the transition as L_z increases, T_c also decreases. It is therefore important to note that there is another length in the problem [2]

$$\Lambda(T) \equiv \phi_0^2/8\pi T = (2\pi^2 J_0/T)\kappa\lambda. \qquad (12)$$

For our simulation, we have $30 = L_z \ll \Lambda(T_m) \simeq 410$.

It has been argued [14] that Λ determines the length on which phase correlations $C(\mathbf{r}) \equiv \langle e^{i[\theta(\mathbf{r})-\theta(0)]}\rangle$ decay in the vortex line lattice; however, these same calculations show that in the vortex liquid the decay length of $C(\mathbf{r})$ is comparable to the spacing between vortex lines $a_v \ll L_z$. Thus this analysis of $C(\mathbf{r})$ does not indicate why Λ should be an important length above T_m, where we continue to see superconducting coherence.

Another possibility is suggested by Nelson's analogy [1] between vortex lines and the imaginary time world lines of 2D bosons. Nelson argued that there should be a Kosterlitz-Thouless (KT) superfluid transition of the analog bosons. For L_z sufficiently large, this KT transition would occur at a $T_c < T_m$, and so would be preempted by the formation of the vortex line lattice. But for L_z small enough, $T_c > T_m$, and one has a new state intermediate between the vortex line lattice and the normal vortex line liquid [15]. We now restate our earlier calculation [11] of this T_c in order to show that the length which distinguishes between these two possibilities is $\Lambda(T_m)$.

As shown by Pollock and Ceperley [16], the 2D boson superfluid density can be expressed in terms of the "winding number" $\mathbf{W}$ which is the net spatial distance traveled by the ensemble of bosons as they travel down the time axis of their world lines. One has $\rho_s^{\text{boson}} = mT_{\text{boson}}\langle W^2\rangle/2\hbar^2$. According to the KT theory, the 2D superfluid transition occurs at a universal value of ρ_s^{boson}, which translates into the condition $\langle W_c^2\rangle = 4/\pi$. In terms of vortex lines, $\mathbf{W}$ just measures the net vorticity transverse to $\mathbf{H}$ [11]. We thus have [17]

$$\langle W_y^2\rangle = \lim_{q_x \to 0} \frac{1}{L_\perp^2}\langle n_y(q_x)n_y(-q_x)\rangle. \qquad (13)$$

This is precisely the same correlation as enters Υ_z, and, comparing with Eq. (7), we can write $\gamma_z = 1 - [\Lambda(T)/L_z]\langle W_y^2\rangle$. Thus $\rho_s^{\text{boson}} \propto \langle W^2\rangle = 0$ implies $\gamma_z = 1$; the normal boson fluid corresponds to a vortex line liquid with coherence along $\mathbf{H}$. $\rho_s^{\text{boson}} > 0$ implies $\gamma_z < 1$; the boson superfluid corresponds to the normal vortex line liquid [18].

We have shown [11] that for a normal vortex line liquid, $\langle n_y(q_x)n_y(-q_x)\rangle = f^2 L_\perp^2 L_z T/c_{44}(q_x)$, where $c_{44}(0) = (B^2/4\pi)dH_x/dB_x$ is the tilt modulus, and $f = B/\phi_0$. Thus we conclude that $\langle W^2\rangle = \langle W_x^2 + W_y^2\rangle = 2\langle W_y^2\rangle = (8\pi L_z T/\phi_0^2)dB_x/dH_x$. This yields

$$T_c = \frac{\phi_0^2}{2\pi^2 L_z}\frac{dH_x}{dB_x} \quad \text{or} \quad \frac{T_c}{T_m} = \frac{4}{\pi}\frac{\Lambda(T_m)}{L_z}\frac{dH_x}{dB_x}. \qquad (14)$$

For large $B \gg H_{c1}$, $dH_x/dB_x \simeq 1$. Thus for $L_z < (4/\pi)\Lambda(T_m)$, one has $T_c > T_m$ and hence a vortex line liquid with superconducting coherence along **H**, intermediate between the vortex line lattice, and the normal vortex line liquid. Only for $L_z > (4/\pi)\Lambda(T_m)$ will this intermediate state disappear [19]. For YBCO, with $T_m \simeq 90$ K, one has $\Lambda(T_m) \simeq 1400$ μm, much thicker than the samples (~ 50 μm) in Refs. [3,4,13].

We note that for $B \gg H_{c1}$, $\Lambda(T_m)$ is a factor B/H_{c1} larger than the "entanglement" length originally proposed by Nelson [1] as the criterion for the 2D boson superfluid transition. This is because the notion of superfluidity, as measured by **W**, does not precisely correspond to the geometric notion of line entanglement. If just as many lines wander to the right as wander to the left, one has **W** = 0, although the lines may still be quite twisted and geometrically entangled.

Finally, we note that for our model Eqs. (12) and (14) would predict $T_c = (8\pi J_0 \kappa \lambda/L_z)T_m \simeq 25$, much higher than the observed $T_c \simeq 2.0$. We believe that this results from a breakdown of the boson analogy near our observed T_c, due to the proliferation of thermally excited closed vortex rings, and intersections between vortex lines, such as cause the transition in a $B = 0$ model. This is clearly the case for the $\lambda \longrightarrow \infty$ model [8], where $\lambda \longrightarrow \infty$ at fixed J_0 also means $\Lambda \longrightarrow \infty$. Equation (14) would then imply $T_c \longrightarrow \infty$. The finite T_c found in $\lambda \longrightarrow \infty$ simulations [8] therefore indicates such a breakdown of the boson analogy. Our present results concerning vortex ring distributions and line intersections are similar to what was found for $\lambda \longrightarrow \infty$ [8].

To conclude, we find from simulations with $\lambda \ll L_z \ll \Lambda(T_m)$ (as is the case for recent experiments) that superconducting coherence parallel to **H** persists into the vortex line liquid state. We argue that this effect should vanish once $\Lambda(T_m) \leq L_z$.

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