Vortex Entanglement in High-T_c Superconductors

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New kinds of intermediate flux states should be accessible in high-T_c superconductors, in fields slightly above H_{c1}. Flux-line wandering leads to an entangled vortex state whose statistical mechanics is isomorphic to an interacting 2D Bose superfluid with cooperative ring exchanges. In sufficiently thin samples, this "braided flux" phase transforms into a liquid of disentangled rods.

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One of the many fascinations of the CuO_2-based superconductors[1] is the possibility of novel fluctuation effects due to the high critical temperatures and small coherence lengths. Interesting modifications of the standard BCS-based Ginzburg-Landau mean-field theory may be expected at T_c in zero field,[2] and when the Abrikosov flux lattice forms with decreasing temperatures at H_{c2}.[3]

In this paper it is shown that there are also remarkable fluctuation effects near H_{c1}, where well-separated flux lines first penetrate the Meissner phase with increasing applied field H. The striking high-resolution Bitter decorations of hexagonally correlated flux quanta in $YBa_2Cu_3O_7$ of Gammel *et al.*[4] provide strong evidence of flux penetration in an intermediate state, regardless of the underlying microscopic mechanism[1] for the superconductivity. Because of the large critical temperatures, flux lines can wander significantly as they traverse a sample of thickness L, in contrast to the rigid vortex lines assumed in the classic Abrikosov treatment of the intermediate state.[5] This line wandering changes the nature of the transition at H_{c1}, and leads to new physics for $H \gtrsim H_{c1}$.

My starting point is the Gibbs free energy for N flux lines whose positions with a field H along the z direction in a sample length L are given by $\mathbf{r}_i(z)=(x_i(z),y_i(z))$, $i=1,\ldots,N$. I work in the London limit, since the ratio of the penetration depth λ to the coherence length ξ is typically quite large, $\kappa=\lambda/\xi \approx 10^2$. If ϵ_1 is the energy per unit length of a single flux line, and $\Phi_0=2\pi\hbar c/2e$ is the flux quantum, the energy reads[5]

$$G=\left(\epsilon_1-\frac{H\Phi_0}{4\pi}\right)NL+\frac{\Phi_0^2}{8\pi^2\lambda^2}\sum_{i>j}\int_0^L K_0(\mathbf{r}_{ij}(z)/\lambda)dz+\tfrac{1}{2}\epsilon_1\sum_{i=1}^{N}\int_0^L\left|\frac{d\mathbf{r}_i(z)}{dz}\right|^2 dz, \quad (1)$$

where $\mathbf{r}_{ij}=\mathbf{r}_i-\mathbf{r}_j$ and $K_0(x)$ is the modified Bessel function, $K_0(x)\approx(\pi/2x)^{1/2}e^{-x}$ for large x. The last term comes from the expansion of the total line energy, $E_i=\epsilon_1\int_0^L(1+|d\mathbf{r}_i/dz|^2)^{1/2}dz$. Flux lines begin to penetrate when the first term changes sign, i.e., when $H\geq H_{c1}-4\pi\epsilon_1/\Phi_0$. Conventional treatments of the transition at H_{c1} assume that the vortices form a triangular lattice of rigid rods with areal density $n=B/\Phi_0$ parallel to the z axis, so that the last term of (1) vanishes. Balancing the first two terms then leads to[5]

$$B=\frac{2\Phi_0}{\sqrt{3}\lambda^2}\left\{\ln\left[\frac{3\Phi_0}{4\pi\lambda^2(H-H_{c1})}\right]\right\}^{-2}, \quad (2)$$

for H close to H_{c1}.

The treatment sketched above neglects thermal fluctuations in the vortex positions as they traverse the length of the sample. A simple random-walk argument shows that the root mean square distance traveled perpendicular to the field is of order $\Lambda_L=(2\pi L k_B T/\epsilon_1)^{1/2}$. Although this quantity is small in conventional superconductors, it is an order of magnitude larger in $YBa_2Cu_3O_7$, because of the high T_c's and relatively modest H_{c1}'s. If we take for concreteness $T=77$ K, $H_{c1}(77\text{ K})=70$ g, and $L=1$ cm, we find that $\Lambda_L=(8\pi^2 L k_B T/\Phi_0 H_{c1})^{1/2}=2.5$ μm. Just as in treatments of wall wandering in 2D commensurate-incommensurate transitions,[6] collisions between vortex lines will be important whenever Λ_L becomes comparable to the line spacing $d\approx(\Phi_0/B)^{1/2}=n^{-1/2}$.

To estimate how collisions alter the prediction (2) in the limit of large sample sizes, note first that a full statistical treatment of (1) entails integration of $\exp(-G/k_B T)$ over all vortex trajectories $\{\mathbf{r}_i(z)\}$. Following Ref. 6, note that each collision reduces the entropy in this sum relative to a noninteracting system by $k_B\ln q$, with $q>1$. Since the spacing between collisions in the z direction is roughly $l=\epsilon_1/k_B T n$, the total number of collisions is of order $(L/l)N=(LA)n^2 k_B T/\epsilon_1$, where A is the cross-sectional area. The statistically averaged Gibbs free energy per unit volume $g(n)$ acquires an entropic contribution

$$g(n)=g_0+(\epsilon_1-H\Phi_0/4\pi)n+n(3\Phi_0^2/8\pi^2\lambda^2)K_0(d/\lambda)+(k_B T)^2 n^2(\ln q)/\epsilon_1. \quad (3)$$

Here, g_0=const and only the contribution from the six nearest neighbors has been used to estimate the second term of (1). Upon minimization with respect to n, the third term dominates the second for small $n=B/\Phi_0$ and one finds $B \approx c[\epsilon_1 \Phi_0^2/(k_B T)^2](H-H_{c1})$ where c is a geometrical constant.

Although there are logarithmic corrections to this result (see below), it is already apparent that wall wandering can produce important changes in the rigid-rod theory. Upon equating the above prediction with Eq. (2), neglecting logarithms but using a more accurate estimate of c given below, we find that wall collisions change the nature of the transition at H_{c1} when

$$(H-H_{c1})/H_{c1} \lesssim \delta h_c = (8\pi/\sqrt{3})(k_B T/\lambda \epsilon_1)^2.$$

The parameters used above (with $\lambda = 2000$ Å) give $\delta h_c = 0.3\times 10^{-5}$. Although this reduced field is small, considerably larger values can be obtained by one's working closer to T_c, since ϵ_1 vanishes like λ^{-2} in this limit.[5]

Fluctuations not only change the nature of the transition at H_{c1}, they also produce new phases for $H > H_{c1}$. To see this the partition function associated with Eq. (1) must be treated more carefully. It will be convenient to impose periodic boundary conditions in the z direction: A configuration of vortices in the plane $z=0$ must lead to an identical configuration when lines reach the plane $z=L$. To sample the allowed phase space completely, one must sum over different ways of connecting the vortices between these two planes. The partition function is thus

$$Z = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_P \int_{\mathbf{r}_1(0)}^{P[\mathbf{r}_1(0)]} d^3 r_1(z) \cdots \int_{\mathbf{r}_N(0)}^{P[\mathbf{r}_N(0)]} d^3 r_N(z)\, e^{-G/k_B T}, \quad (4)$$

where there is sum both over N and over permutations P which connect the particles in the two planes.

In this form, the partition function is identical to the Feynman path integral[7] for the grand canonical partition function of a fluid of interacting bosons in two dimensions with chemical potential $\mu = H\Phi_0/4\pi - \epsilon_1$. The trajectories of vortices along $\hat{z}$ are isomorphic to boson world lines.[8] The thermal energy $k_B T$ plays the role of $\hbar$, while the sample thickness L corresponds to the distance $\beta\hbar$ in the imaginary time direction. The vortex line energy ϵ_1 is the boson mass. $\Lambda_L = (2\pi L k_B T/\epsilon_1)^{1/2}$ is a classical analog of the thermal de Broglie wavelength.

I first discuss the behavior of the flux lines as $L \to \infty$, where the problem reduces to that of finding the ground state of interacting bosons in two dimensions. Both the boson "masses" ϵ_1 and interaction range λ are adjustable by variation of the temperature of the superconducting sample. Just as zero-point energy can melt a crystal of light bosons at sufficiently low pressures, the usual Abrikosov flux-lattice state will be melted by thermal wall wandering at fields H such that the spacing between flux lines exceeds λ. To estimate the field H_x below which the flux lattice becomes "superfluid," I assume a density of lines such that (2) holds. The flux-line spacing will equal the range of interactions when $B=\Phi_0/\lambda^2$, which leads to the estimate

$$H_x - H_{c1} \approx (3\Phi_0/4\pi\lambda^2)\exp(-2^{1/2}/3^{1/4}).$$

Using the result[5] $H_{c1} = \Phi_0(\ln\kappa)/4\pi\lambda^2$, I find that the superfluid exists over a reduced field range

$$(H_x - H_{c1})/H_{c1} = (3/\ln\kappa)\exp(-2^{1/2}/3^{1/4}) = 0.22$$

for $\kappa = 10^2$.

The chemical potential μ of the 2D Bose gas is known to be related to the particle density n by[9] $\mu = (4\pi n\hbar^2/m)/|\ln(na^2)|$, where a is the interaction range. Upon translating this result into the language of type-II superconductors, I find

$$B \approx [\epsilon_1 \Phi_0^2/16\pi^2 (k_B T)^2](H-H_{c1})\,|\ln[\epsilon_1 \Phi_0 (\lambda/4\pi k_B T)^2 (H-H_{c1})]|. \quad (5)$$

Except for the logarithmic correction, this has the form predicted by my naive random-walk argument, with $c = 1/16\pi^2$. The logarithm appears because particles occasionally slip past each other instead of colliding. There is also a singular term in the Gibbs free energy, $G(H,T) \sim (H-H_{c1})^2 \ln(H-H_{c1})$, which implies a logarithmic divergence in the specific heat $C_H(T)$ as H_{c1} is approached from high temperatures. In addition to the behavior implied by Eq. (5), the B vs H curve will have a jump at $H_x(T)$, if, as seems likely, the transition from a flux crystal to a superfluid liquid is first order.

What does superfluidity mean for a liquid of flux lines? To answer this question, assume $L < \infty$, and consider the phase diagram shown in the inset to Fig. 1, drawn for 2D bosons with a purely repulsive potential, as a function of "chemical potential" $(H-H_{c1})$ and "temperature" (L^{-1}). The real temperature is held fixed at $T < T_c$. For small L and low line densities, Λ_L is much less than $n^{-1/2}$, and we have a "disentangled flux liquid" (phase B) of lines which do not meander significantly as they traverse the sample. As L becomes larger, particles begin to trade places with appreciable probability, leading eventually to arbitrarily large cooperative ring exchanges[7] in the superfluid phase (A). This elegant picture of the transition has been confirmed numerically for

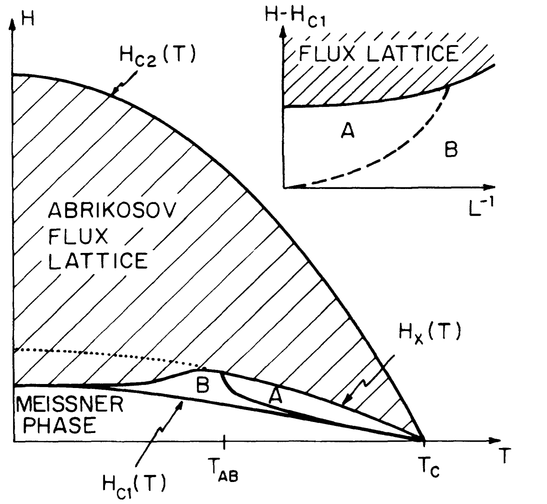

FIG. 1. Abrikosov flux lattice (shaded), entangled-flux liquid (A), and disentangled-flux liquid (B) phases as a function of H, T, and L^{-1}.

He[4] by Ceperley and Pollock in both three and two dimensions.[10] Its meaning here is that the liquid of flux lines becomes "braided" or entangled below the superfluid transition. Although averaging over different connections of lines with periodic boundary conditions only approximates the free boundary conditions appropriate for vortex lines in a superconductor, this difference in boundary conditions will clearly not affect the "entangled flux liquid" when $L \to \infty$. I expect, moreover, that entanglement will persist for large but finite L even with free boundary conditions.

The above arguments suggest the existence of a sharp transition from phase A to phase B in a superconductor. Assuming for simplicity that a transition exists, and that it is a Kosterlitz-Thouless transition, we can again transcribe results for 2D Bose fluids,[9] and find that the critical thickness for dilute vortex densities n is $L_c = (\epsilon_1/2\pi k_B T n)\ln\ln(1/n\lambda^2)$, a result which becomes exact when $\ln\ln(1/n\lambda^2) \gg 1$. For $T = 77$ K, $H_{c1} = 70$ g, and $n^{-1/2} = 4\times 10^{-5}$ cm, I neglect the logarithm and find $L_c \approx \Phi_0 H_{c1}/8\pi^2 n k_B T = 0.26$ mm. In general, the entangled vortex liquid appears at line densities such that

$$\lambda \lesssim n^{-1/2} \lesssim \Lambda_L = (32\pi^3 k_B T L/\Phi_0 \ln\kappa)^{1/2}\lambda.$$

A guess for the phase diagram based on these inequalities is shown in Fig. 1, for a sample of fixed thickness L. Phase A terminates below a temperature $T_{AB} \approx \Phi_0^2(\ln\kappa)/32\pi^3 L k_B$, where these inequalities are first violated. $T_{AB} \approx 14$ K for a 1-mm sample with $\kappa = 10^2$. When $L \to \infty$, phase B disappears, and the superfluid phase A is separated from the flux crystal by the dotted continuation of the line $H_x(T)$.

Bitter patterns alone[4] are not enough to distinguish phases A and B. Vortex cores will display liquidlike order in any constant-z cross section of both the entangled- and disentangled-flux liquids. These phases should have markedly different signatures, however, when correlations among the flux lines are probed by neutron scattering.[5] In the disentangled-flux liquid, diffuse rings of scattering in the (q_x, q_y) plane will be sharp along q_z. In the entangled-flux liquid, on the other hand, these rings will be *diffuse* along q_z because of short-range correlations along $\hat{\mathbf{z}}$ induced by entanglement. Neutron scattering might also uncover other phases, such as hexatic liquid of flux lines, which could become entangled just as in phase A.

The response of the flux-flow resistivity to pinning should also differ in phases A and B. Strong pinning could, of course, destroy any of the phases discussed above, including the Abrikosov flux lattice. Tinkham, however, has argued that the ratio of the pinning energy to $k_B T_c$ in $YBa_2Cu_3O_7$ is 25 times smaller than in, e.g., Nb_3Sn,[11] so that pinning should be rather weak at the elevated temperatures of phase A. Weak pinning by dilute concentrations of defects could still suppress flux flow in phase A, because one securely pinned line will entangle many of its neighbors. Pinning of the disentangled lines in the B phase should be much less effective. Strong pinning at low temperatures could lead to *quenched* analogs of the A and B phases: Kardar and Zhang[12] have shown that an isolated flexible line in a random medium wanders even more strongly than its thermal counterpart, $\langle |\Delta r|^2\rangle^{1/2} \sim L^{0.6}$. This may be the explanation of the liquidlike order of the flux patterns of Ref. 4, which were taken at 4.2 K. The lack of any observed patterns at 77 K, on the other hand, may be due to time-dependent flux line wandering in an equilibrated A or B phase.

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Note added.— Although this analysis has been restricted to the vicinity of H_{c1}, there may also be fluctuation-induced flux-lattice melting phenomena in the vicinity of H_{c2}, as has been seen in recent experiments by D. J. Bishop, P. L. Gammel, L. F. Schneemeyer, and J. V. Waszczak.[13]

[1]M. Rice, Z. Phys. B **67**, 141 (1987), and references therein.
[2]C. Dasgupta and B. I. Halperin, Phys. Rev. Lett. **47**, 1556 (1981).
[3]E. Brézin, D. R. Nelson, and A. Thiaville, Phys. Rev. B **31**, 7124 (1985).
[4]P. L. Gammel, D. J. Bishop, G. J. Dolan, J. R. Kwo, C. A. Murray, L. F. Schneemeyer, and J. V. Waszczak, Phys. Rev. Lett. **59**, 2592 (1987).
[5]A. L. Fetter and P. C. Hohenberg, in *Superconductivity*, edited by R. D. Parks (Dekker, New York, 1969), Vol. 2.

[6]S. N. Coppersmith, D. S. Fisher, B. I. Halperin, P. A. Lee, and W. F. Brinkman, Phys. Rev. B **25**, 349 (1982).

[7]R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965), pp. 287–294.

[8]A similar analogy has been used for interacting lines in $d=2$ by P. G. de Gennes, J. Chem. Phys. **48**, 2257 (1968). Although the mapping here is onto noninteracting fermions, this system is equivalent to an *interacting* 1D Bose gas. For a related dimer problem in 2+1 dimensions, see S. M. Bhattacharjee, J. F. Nagle, D. A. Huse, and M. E. Fisher, J. Stat. Phys. **32**, 361 (1983).

[9]M. Schick, Phys. Rev. A **3**, 1067 (1971); V. N. Popov, Theor. Math. Phys. (Engl. Transl.) **11**, 565 (1972); D. S. Fisher and P. C. Hohenberg, Phys. Rev. B (to be published).

[10]D. M. Ceperley and E. L. Pollock, Phys. Rev. Lett. **56**, 351 (1986); E. L. Pollock and D. M. Ceperley, Phys. Rev. B **36**, 8343 (1987), and to be published.

[11]M. Tinkham, Helv. Phys. Acta (to be published).

[12]M. Kardar and Y.-C. Zhang, Phys. Rev. Lett. **58**, 2087 (1987).

[13]D. J. Bishop, private communication.