

## Superconducting coherence and the helicity modulus in vortex line models

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We show how commonly used models for vortex lines in three-dimensional superconductors can be modified to include  $\mathbf{k}=\mathbf{0}$  excitations. We construct a formula for the  $\mathbf{k}=\mathbf{0}$  helicity modulus in terms of fluctuations in the projected area of vortex loops. This gives a convenient criterion for the presence of superconducting coherence. We also present Monte Carlo simulations of a continuum vortex line model for the melting of the Abrikosov vortex lattice in pure YBCO. [S0163-1829(99)12213-6]

Phase transitions involving vortices in high-temperature superconductors are the subject of intense study both experimentally and theoretically.<sup>1</sup> The enhanced thermal fluctuations strongly alter large parts of the mean-field phase diagram,<sup>2,3</sup> with new phases appearing, e.g., vortex line liquids, vortex glass phases, etc. A convenient quantity to study theoretically is the helicity modulus  $Y$  (or spin-wave stiffness), which measures the free-energy increment associated with an externally imposed twist in the phase of the superconducting order parameter,<sup>4</sup> and is proportional to the macroscopic superfluid density. Much work has been based on  $XY$ -like models, defined in terms of this phase, where vortices appear only as topological defects. However, a formulation directly in terms of vortex degrees of freedom has several advantages. In this paper we show how the uniform helicity modulus can be defined directly in terms of the vortex lines, without reference to the phase. We also show Monte Carlo results for  $Y$  and other quantities in a continuum model of interacting vortex lines.

One of the advantages of the vortex representation is the possibility to define the model on a continuum, and so avoid artificial pinning to a discretization lattice. Furthermore, one may include interactions coupling directly to the vortex lines, such as core energies and various types of disorder. The vortex representation therefore allows new parameter regimes to be reached compared to the phase representation. Both representations are frequently used in computer simulations.<sup>5-8</sup>  $Y$  is straightforward to calculate in the phase representation.<sup>5</sup> However, in the vortex representation usually only  $\mathbf{k}\neq\mathbf{0}$  fluctuations are included, making the uniform response  $Y$  exactly zero, and extrapolations from finite  $\mathbf{k}$  become necessary.<sup>6</sup> Furthermore, when screening from gauge field fluctuations is taken into account,  $Y(\mathbf{k})\sim k^2$  for small, but finite  $\mathbf{k}$ , since an imposed phase twist can be compensated by the gauge field. Extrapolation to  $\mathbf{k}=\mathbf{0}$  then gives zero, but the small- $\mathbf{k}$  behavior of  $Y(\mathbf{k})$  may still be related to the Meissner effect in a superconductor and used to detect phase transitions.<sup>6</sup> The methods mentioned above involve extrapolations from the smallest available wave vectors to  $\mathbf{k}=\mathbf{0}$ , thereby severely complicating the data analysis. An alternative may be to study winding number fluctuations, which are related to the magnetic permeability  $\mu$ , but they suffer from being difficult to equilibrate for large system sizes.

In this paper we take a different route by modifying the vortex model in order to incorporate fluctuations with zero wave vector. The form of this modification is obtained using a duality transformation between the phase and vortex representations, paying due attention to the role of the boundary conditions. We show that periodic boundary conditions for the phases enter as an additional term in the Hamiltonian of the vortex representation. This allows direct evaluation of the  $\mathbf{k}=\mathbf{0}$  helicity modulus in terms of fluctuations of the total net area of vortex loops, which can indeed be finite also in the presence of screening. The role of boundary conditions in the duality transformation has previously been explored in two-dimensional (2D) lattice models<sup>9-11</sup> and 3D gauge glass models.<sup>12</sup> Here we generalize this idea to continuous 3D systems, with finite magnetic field, penetration depth, and temperature. Furthermore, we report on Monte Carlo simulations of a continuum London model. In contrast to previous continuum simulations, which used 2D Bose models with planar interaction,<sup>8</sup> we take into account the full 3D long-range interaction. Our model has the essential features to describe the vortex lattice melting transition in pure YBCO, where a continuum description should apply.

The starting point for our discussion is the Ginzburg-Landau theory in the London limit, where amplitude fluctuations of the superconducting order parameter  $\Psi=|\Psi|\exp(i\theta)$  are neglected. For simplicity we will use an isotropic continuum description, since our results are independent of microscopic details. The generalization to other cases is straightforward. The Hamiltonian reads

$$H = \int_{\Omega} d^3\mathbf{r} \left\{ \frac{J}{2} \left( \nabla\theta - \frac{2\pi}{\Phi_0} \mathbf{A} \right)^2 + \frac{\mathbf{B}^2}{8\pi} - \frac{\mathbf{B}\cdot\mathbf{H}}{4\pi} \right\}, \quad (1)$$

where  $\Omega=L_xL_yL_z$  is the size of the system,  $\theta(\mathbf{r})$  is the phase of the superconducting order parameter,  $\mathbf{B}=\nabla\times\mathbf{A}$  is the magnetic flux density,  $\mathbf{H}$  is an externally applied magnetic field,  $\Phi_0=hc/(2e)$  is the flux quantum, and  $J=\Phi_0^2/(16\pi^3\lambda_0^2)$  is a coupling constant with  $\lambda_0$  the bare magnetic penetration depth. The first term in Eq. (1) is the kinetic energy with the superfluid velocity  $\mathbf{v}=\nabla\theta-(2\pi/\Phi_0)\mathbf{A}$ , while the second describes the magnetic energy. The partition function is obtained by integrating over the phases  $\theta(\mathbf{r})$ , and gauge field  $\mathbf{A}(\mathbf{r})$ , subject to some gauge fixing condition:  $Z=\int \mathcal{D}\theta\mathcal{D}'\mathbf{A} e^{-\beta H}$ . In order to get a finite result a short-distance regularization has to be imposed, e.g., by de-

fining the model on a lattice. Physically this cutoff is of the order of the Ginzburg-Landau coherence length  $\xi_0$ , and gives the size of the vortex cores.

We now discuss the transformation of the model, Eq. (1), to a system of interacting vortex lines in some detail. For simplicity we start by considering the case without any externally applied magnetic field,  $\mathbf{H}=0$ . The interaction can be linearized by an integration over an auxiliary field  $\mathbf{b}(\mathbf{r})$ , upon which the kinetic energy becomes  $\int_{\Omega} d^3\mathbf{r} J(i\mathbf{b}\cdot\mathbf{v} + \frac{1}{2}\mathbf{b}^2)$ . The superfluid velocity splits into a longitudinal part, describing the smooth spin-wave fluctuations of the order parameter, and a transverse part describing the singular vortices:  $\mathbf{v}=\mathbf{v}_{\parallel}+\mathbf{v}_{\perp}$ . Integrating over the longitudinal part leads to the constraint  $\nabla\cdot\mathbf{b}=0$ , which can be enforced by setting  $\mathbf{b}=\nabla\times\mathbf{a}$ . After a partial integration of the first term and subsequent integration over  $\mathbf{B}$  the Hamiltonian becomes

$$H = \int_{\Omega} d^3\mathbf{r} J \left\{ 2\pi i \mathbf{a}\cdot\mathbf{m} + \frac{1}{2}(\nabla\times\mathbf{a})^2 + \frac{1}{2\lambda_0^2}\mathbf{a}_{\perp}^2 \right\}, \quad (2)$$

where  $\mathbf{a}_{\perp}$  is the transverse part of  $\mathbf{a}$  and  $\mathbf{m}(\mathbf{r})$  denotes the vorticity,  $\nabla\times\nabla\theta=2\pi\mathbf{m}$ . Integrating out the auxiliary field  $\mathbf{a}$  leaves us with the vortex Hamiltonian<sup>13,6,1</sup>

$$H = \int_{\Omega} \frac{K}{2} \mathbf{m}(\mathbf{r})\cdot V(\mathbf{r}-\mathbf{r}')\mathbf{m}(\mathbf{r}') d^3\mathbf{r} d^3\mathbf{r}', \quad (3)$$

where  $K=(2\pi)^2J$  and  $V$  is the London interaction

$$V(\mathbf{r}) = \frac{1}{\Omega} \sum_{\mathbf{k}} \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\mathbf{k}^2 + \lambda_0^{-2}}, \quad (4)$$

$k_{\mu}=2\pi n_{\mu}/L_{\mu}$ ,  $n_{\mu}\in\mathbb{Z}$ ,  $\mu=x,y,z$ . With periodic boundary conditions for the phases  $\theta$  we also get the constraint of zero net vorticity  $\int_{\Omega}\mathbf{m}(\mathbf{r})d^3\mathbf{r}=0$ .

In going from Eq. (1) to Eq. (2) we implicitly assumed that  $\mathbf{v}$  had no  $\mathbf{k}=0$  component, allowing us to throw away a surface integral. However, if the phases obey periodic boundary conditions,  $\theta(\mathbf{r}+\mathbf{L}_{\mu})=\theta(\mathbf{r})$  (where  $\mathbf{L}_{\mu}=L_{\mu}\mathbf{e}_{\mu}$ ), there will be an additional energy term, coming from uniform fluctuations of  $\mathbf{v}$ . An important point here is that the integration over  $\mathbf{A}$  should not include the uniform part  $\mathbf{A}_0$ , since such fluctuations correspond to fluctuations in the boundary conditions. The additional energy is simply  $H'=(J/2\Omega)\mathbf{v}_0^2$ , with  $\mathbf{v}_0=\int_{\Omega}\mathbf{v}(\mathbf{r})d^3\mathbf{r}$ . This is now related to the vortices as follows. The contribution to the vorticity  $\mathbf{m}$  from a single vortex loop can be written

$$\mathbf{m}(\mathbf{r}) = \oint_{\Gamma} \delta(\mathbf{r}-\mathbf{r}')d\mathbf{r}' = \nabla\times\int_S \delta(\mathbf{r}-\mathbf{r}')d\mathbf{S}', \quad (5)$$

where  $\Gamma$  is a contour describing the vortex loop, and  $S$  denotes an oriented surface which has  $\Gamma$  as a boundary. Summing over all vortex loops gives the total vortex density. Now, since the vorticity is the rotation of the superfluid velocity, we may define

$$\mathbf{Q} = \frac{1}{2\pi} \int_{\Omega} \mathbf{v} d^3\mathbf{r} = \sum_i \int_{S_i} d\mathbf{S}_i, \quad (6)$$

where the sum is over all vortices. This has the interpretation of the total projected net area of the vortex loops in each

direction. Due to the periodic boundary conditions, the value of  $\mathbf{Q}$  is uniquely determined by the positions of the vortices only up to an integer multiple of  $\Omega/L_{\mu}$ , reflecting the need to specify the total phase twist of the system. *Thus the variable  $\mathbf{Q}$  keeps track of the total phase twist of the system and must be independently specified in addition to the vortices in order to completely specify the state of the system.* The additional  $\mathbf{k}=0$  component of the energy is now given by

$$H' = K \frac{\mathbf{Q}^2}{2\Omega}, \quad (7)$$

and the total Hamiltonian is given by the sum of Eqs. (3) and (7):  $H_{\text{tot}}=H+H'$ .

*External magnetic field.* Assume now that  $n$  flux quanta  $\Phi_0$  penetrates the system in the  $z$  direction. In this case the periodic boundary conditions for the phases have to be changed so that the system can accommodate a net number of vortices. For the vortices penetrating the whole system the area  $\mathbf{Q}$  should now be measured with respect to a given reference line at some arbitrary but fixed position determined by the boundary conditions. A possible choice is to let  $\theta(\mathbf{r}+\mathbf{L}_{\mu})-\theta(\mathbf{r})=n\pi-(2\pi/\Phi_0)\int_{\mathbf{r}}^{\mathbf{r}+\mathbf{L}_{\mu}}\mathbf{A}\cdot d\mathbf{r}'$ , with the integral taken along a straight line across the system. In the gauge  $\nabla\cdot\mathbf{A}=0$  we may write  $\mathbf{A}(\mathbf{r})=\mathbf{A}_{\text{per}}(\mathbf{r})+\frac{1}{2}\bar{\mathbf{B}}\times(\mathbf{r}-\mathbf{r}_0)$ , where  $\mathbf{A}_{\text{per}}$  satisfy periodic boundary conditions and  $\bar{\mathbf{B}}=n\Phi_0\mathbf{L}_z/\Omega$  is the uniform part of the flux density. In this case the fixed reference line goes through  $\mathbf{r}_0$  in the direction of  $\bar{\mathbf{B}}$ .

*Helicity modulus.* The full importance of the new term in the energy becomes evident when one considers the superfluid response of the system. Replacing the boundary conditions by twisted,  $\theta(\mathbf{r}+\mathbf{L}_{\mu})\rightarrow\theta(\mathbf{r}+\mathbf{L}_{\mu})+\Theta$ , leads to the replacement  $Q_{\mu}\rightarrow Q_{\mu}-\tilde{A}_{\mu}$  with  $\tilde{A}_{\mu}=\Omega\Theta/L_{\mu}$  in Eq. (7). This allows us to define the zero wave vector helicity modulus by

$$Y_{\mu} = \frac{\Omega}{K} \frac{\partial^2 F}{\partial \tilde{A}_{\mu}^2} = 1 - \frac{K}{\Omega T} \langle\langle Q_{\mu}^2 \rangle\rangle, \quad (8)$$

where  $\langle\langle Q^2 \rangle\rangle = \langle Q^2 \rangle - \langle Q \rangle^2$ , and  $F=-T\ln Z$  is the free energy.  $Y$  is nonzero in the superconducting state and vanishes at the phase transition. In the critical region of a continuous phase transition it obeys the Josephson scaling relation  $Y\sim\xi^{-1}$ , where  $\xi(T)$  is the correlation length.<sup>4</sup>

The ordinary vortex Hamiltonian, Eq. (3), without the additional area term  $H'$  is recovered by integrating over  $\Theta$  and thus corresponds to having fluctuating boundary conditions.<sup>9</sup> In this case the  $\mathbf{k}=0$  response is zero. Fluctuations in the winding number  $\mathbf{W}=\int_{\Omega}\mathbf{m}(\mathbf{r})d^3\mathbf{r}$ , are obtained only if the  $\mathbf{k}=0$  component of the magnetic flux density  $\mathbf{B}$  is allowed to fluctuate. Then the magnetic permeability  $\mu_{\nu}=4\pi\partial\langle B_{\nu} \rangle/\partial H_{\nu}=\langle\langle B_{\nu}^2 \rangle\rangle/\Omega T=\langle\langle W_{\nu}^2 \rangle\rangle\Phi_0^2/\Omega T$  can be calculated.

*Monte Carlo simulations.* To clearly demonstrate the practical usefulness of these ideas we now discuss Monte Carlo (MC) simulations. The inclusion of the area term in a simulation is straightforward. With the model defined in terms of vortices, the Monte Carlo moves consist of deformations of the vortex lines and (possibly) creations and destructions of closed loops. The change in the projected area coming from these local updates are accumulated in  $\mathbf{Q}$ , and

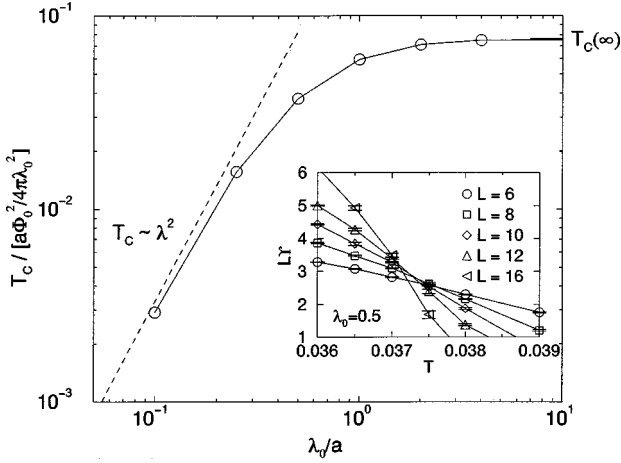


FIG. 1. Monte Carlo results for the  $(\lambda_0, T)$  phase diagram for  $\mathbf{B}=0$ . The dotted line indicates the value of  $T_c$  for the inverted XY model obtained in the limit  $\lambda_0 \rightarrow 0$ ,  $T_c \approx Ka(\lambda_0/a)^2/3.0$  ( $a$  is the lattice constant  $\sim \xi_0$ ). In the opposite limit,  $\lambda_0 \rightarrow \infty$ ,  $T_c \approx 3.0Ka/(2\pi)^2$ . Inset:  $T_c$  is located at the intersection of curves for  $LY$  for different  $L$ .

the change in total energy, including the area term Eq. (7), must be used to calculate the transition probabilities of the Markov chain. Optionally, these moves may be supplemented by global moves where  $Q_\mu$  is changed by  $\pm \Omega/L_\mu$ , corresponding to dragging a whole vortex across the entire system. The acceptance ratio for such moves can be expected to be quite low because of the high energies involved. Alternatively these global moves can be integrated out exactly, leading to the replacement of  $H'$  by a periodic Gaussian:  $\exp(-\beta H') \rightarrow \sum_{M_\mu} \exp[-(1/2\Omega T) \sum_\mu K(Q_\mu - M_\mu \Omega/L_\mu)^2]$ .<sup>14</sup> Since this form of the area term leads to a somewhat more complicated expression for the helicity modulus it will not be used in what follows.

We present simulation results for two different models: (i) a lattice superconductor in zero magnetic field with different values of  $\lambda_0$ , (ii) a continuum vortex model of the melting of the Abrikosov vortex lattice. In both cases  $10^5$ – $10^6$  Monte Carlo sweeps were used, with the initial  $\sim 10\%$  discarded for equilibration.

In Fig. 1 we present results from the first case, in which the phase transition is continuous. The critical temperature  $T_c$  is determined from finite size scaling of the helicity modulus  $Y(T, L) = L^{-1} \tilde{Y}[(T - T_c)L^{1/\nu}]$ , as shown in the inset. Due to the new length scale given by  $\lambda_0$ , scaling works only for rather large system sizes and corrections are clearly visible for small sizes, but the determination of  $T_c$  is still quite accurate. In the limits  $\lambda_0 \rightarrow \infty$  and  $\lambda_0 \rightarrow 0$  we recover known results, showing that our method works properly. Furthermore, a scaling collapse of MC data for  $\lambda=0.25$  is obtained using the expected 3D XY value  $\nu \approx 2/3$ .

In our continuum simulations in an applied magnetic field, we discretize the vortex lines only along the  $z$  direction, using straight segments to interpolate between the  $xy$  planes where the positions are continuous. We exclude overhangs and isolated loops, which should be of importance only close to the zero field  $T_c$ . In addition to local MC moves of the positions in the  $xy$  plane, we include moves where two flux lines are cut off and reconnected to each

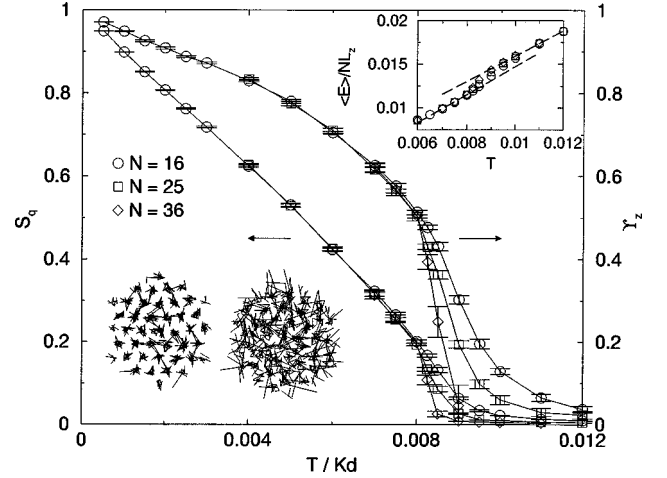


FIG. 2. Helicity modulus  $Y_z$  and structure function  $S_q$  at an ordering vector of the vortex lattice. Inset shows the jump in energy per vortex and layer at the transition. Also shown are two typical snapshots from the simulation: one below, and one above  $T_c \approx 0.008Kd$ .

other, allowing different permutations of the boundary conditions to be sampled. We use a full 3D long-range interaction, given by Eq. (4) (with  $\lambda_0 = \infty$ ), supplemented by a Gaussian short-distance cutoff  $e^{-k^2 \xi_0^2}$ , which acts between the midpoints of the vortex line segments. The vortex lattice constant was set to  $4\xi_0$  and the layer separation  $d$  to  $2\xi_0$ . The number of layers for a system of  $N$  vortices was set to  $4\sqrt{N}$ . To avoid frustration effects in the vortex lattice phase we use a hexagonal simulation cell with periodic boundary conditions in all directions. In Fig. 2 we show the helicity modulus in the direction of the applied field  $Y_z$ , and the structure function  $S_q = \langle |m_z(\mathbf{q})|^2 \rangle / (NL_z)^2$  at a reciprocal vector  $\mathbf{q}$  of the Abrikosov vortex lattice, as a function of temperature.  $Y_x = Y_y = 0$  for all  $T$ , reflecting the absence of vortex pinning. At the transition both  $Y_z$  and  $S_q$  drop quite sharply, suggesting a first-order melting transition to an entangled vortex liquid with no intermediate disentangled phase. Right at the transition, the time series of the internal energy or the structure function, obtained from the simulation, fluctuate around two different values, giving further support for a first-order transition. The inset shows how the average energy per vortex and layer approaches a jump at the transition as system size increases, with a latent heat of roughly  $0.0015NL_z K$ . Taking into account the internal temperature dependence of the parameters,<sup>15</sup> and using values for YBCO gives an entropy jump  $\Delta S \approx 0.5k_B$  per vortex and layer, in rough agreement with experiments.<sup>16</sup>

We now comment on the implications of the ideas presented above on the analogy between the statistical mechanics of vortex systems and zero temperature quantum field theory of bosons in  $(2+1)D$ .<sup>2,17</sup> The vortex lines are the analogue of boson world lines in a path integral representation of the partition function, with the  $z$  direction playing the role of imaginary time. A crystal ground state for the bosons corresponds to the Abrikosov vortex lattice phase in the vortex problem, while a superfluid boson ground state is mapped to an entangled vortex line liquid. The winding number fluctuations of world lines in  $(2+1)D$  gives the su-

perfluid density of the boson problem.<sup>18</sup> It is of interest to study the consequences of our area term  $H'$  in this context. To this end it is useful<sup>19</sup> to view the London interaction, as being mediated by a (massive in the screened case)  $(2+1)D$  gauge field  $a_\mu$ , see Eq. (2). The area term  $H'$  is now generated by integrating over the  $\mathbf{k}=\mathbf{0}$  component of the dual field strength  $\tilde{f}_\mu = \epsilon_{\mu\nu\rho} \partial_\nu a_\rho$  [which corresponds to the auxiliary field  $\mathbf{b}$  above Eq. (2) in the vortex problem]. By coupling the dual field strength  $\tilde{f}_\mu = (e_y, e_x, b_z)$  to an external source  $\tilde{g}_\mu = (d_y, d_x, h_z)$ , we find that the dual magnetic permeability  $\mu = \partial \langle b_z \rangle / \partial h_z$  corresponds to the helicity modulus in  $z$  direction  $Y_z$ .<sup>1,6</sup> The inverse dual dielectric constants  $\epsilon_i^{-1} = \partial \langle e_i \rangle / \partial d_i$  in the  $x$  and  $y$  directions, correspond to the helicity modulus  $Y_\mu$  in the  $y$  and  $x$  directions, respectively.

In summary, we have shown how to include  $\mathbf{k}=\mathbf{0}$  fluctuations in vortex line models, and how the helicity modulus can be obtained from fluctuations of the projected area of vortex loops. This is useful for detecting superconducting phase transitions in models with and without screening of the London interaction. We also presented continuum Monte Carlo simulation results with a full 3D London interaction. This model should be appropriate for the vortex lattice melting in moderately anisotropic systems such as YBCO. Similar approaches should be useful in studies of, e.g., vortex glass transitions and quantum phase transitions.

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