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Crossover from three- to two-dimensional behavior of the vortex energies in layered *XY* models for high-T_c superconductors

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We use Monte Carlo simulations of a layered *XY* model to study phase fluctuations in high-T_c superconductors. A vortex-antivortex interaction dominated by a term linear in the vortex separation is found in the low-temperature regime. This is in agreement with a zero-temperature variational calculation. At temperatures just above the two-dimensional (2D) vortex-unbinding temperature, the linear term vanishes and an ordinary 2D vortex behavior is found. This explains the finding that high-T_c superconductors show 2D properties in the vortex fluctuations responsible for the resistivity transition close to the critical temperature.

High-temperature superconductors exhibit a resistivity transition similar to conventional thin-film type-II superconductors.[1-5] The transition of thin films has been understood in terms of unbinding of thermally activated vortices. A detailed Coulomb-gas scaling theory has been developed and is very successful in describing the resistivity transition in thin films.[6] The very fact that Coulomb-gas scaling also works well for those high-temperature superconductors, taken together with the layered structure of these materials, suggests that the resistivity transition is driven by thermally activated vortices within the individual CuO planes.

A crucial ingredient in the scaling theory is the functional form of the vortex-antivortex interaction. In a Ginzburg-Landau description, the two-dimensional (2D) interaction energy pertinent to thin films has a logarithmic dependence on the separation. The coefficient of the logarithmic term and the core energy of a vortex can be tied together within this description. The Hamiltonian constructed for the vortex gas can be recast into a dimensionless thermodynamical description with all the sample-dependent properties absorbed into the temperature scale. This is the key ingredient of Coulomb-gas scaling and has been well established for thin superconducting films.[6]

The layered *XY* model is a simple model of such a structure of weakly coupled superconducting planes. The intraplane interaction will introduce an extra contribution to the vortex-antivortex interaction. In a zero-temperature variational calculation by Cataudella and Minnhagen,[7] this extra term was found to depend linearly on the vortex separation. The subject of this Rapid Communication is an investigation of the effect of thermal fluctuations, especially vortex excitations, on the vortex-pair interaction.

We have performed Monte Carlo measurements of the vortex energies in two weakly coupled layers of *XY* planes. Our simulations show that the thermal vortex fluctuations decouple the planes at a certain temperature. The decoupling retrieves the 2D functional form of the vortex-antivortex interaction. We parametrize the energy of a vortex-antivortex pair of size a by the following form suggested by the zero-temperature variational calculation by Cataudella and Minnhagen,[7]

$$E(a)=E_c+E_1\ln(a/a_0)+E_2(a/a_0-1)\,, \tag{1}$$

where E_c is the creation energy of a vortex pair at a distance equal to the core diameter a_0 of a vortex. In the Cataudella-Minnhagen calculation, a vortex pair is imposed as a boundary condition in one plane. The energy of the pair is calculated variationally under the condition that the adjacent plane is fixed in the ground state. The logarithmic interaction at short distances is the familiar two-dimensional vortex-pair interaction. The linear contribution is due to the interplane coupling. It is of great interest to study how this zero-temperature result is influenced by thermal fluctuations. We use Monte Carlo simulations to calculate the vortex-pair energy in the case where the adjacent plane is allowed to fluctuate freely, i.e., spin-wave excitations as well as thermally induced vortices are present. In the plane of the imposed vortex pair we restrict the fluctuations to spin waves only.

Our main result is that vortex fluctuations in the adjacent plane makes the coefficient of the linear term in the energy vanish as the temperature increases. As this happens, the vortex-antivortex interaction recovers its usual 2D logarithmic form. This occurs for temperatures just above the vortex unbinding temperature of the 2D *XY* model. This finding might explain how the layered three-dimensional high-temperature superconductors can exhibit 2D Coulomb-gas scaling behavior in the resistivity transition.

The model is defined by the Hamiltonian

$$H_0=J_{\parallel}\sum_{\nu=1}^{2}\sum_{\langle i,j\rangle}\cos(\theta_i^{\nu}-\theta_j^{\nu})+J_{\perp}\sum_{i}\cos(\theta_i^{2}-\theta_i^{1})\,, \tag{2}$$

where $\theta_i^{\nu}\in[0,2\pi)$ is the angle at site i in plane number ν.

The summation $\langle i,j \rangle$ is over nearest neighbors. The coupling $J_\perp$ models the Josephson coupling between the planes in the superconductor.[7] We have periodic boundary conditions along the x and y directions. The variables θ_i^ν are located on the sites of a square lattice in the (x,y) plane.

Our purpose is to study the effect of thermal fluctuations in plane II on the energy of a vortex pair in plane I. We especially want to identify the role played by the vortex fluctuations. Hence, we need to be able to control the density of thermally induced vortices in both places.

In order to control the number of vortices, we modify the original Hamiltonian H_0 to

$$H_1 = H_0 + \sum_{\nu=1}^{2} \lambda^\nu \sum_j |v_j^\nu| , \qquad (3)$$

where v_j^ν is the vorticity at site j in the dual lattice for plane number ν. The values of v_j^ν are ± 1 or 0, λ^ν is a Lagrangian multiplier controlling the vortex density. The vorticity at site j in the dual lattice is defined as the discretized version of the integral along a close loop $(1/2\pi)\oint \nabla\theta \cdot dl$ in the following way: $v_j = (1/2\pi) \times \sum_{i=1}^{4} [(\theta_{i+1} - \theta_i) \text{ (mod) } 2\pi)]$. Here, the site index i runs in the positive direction through the four corners of the smallest square in the direct lattice enclosing the site j of the dual lattice. It is understood that site $i+1=5$ is identical to site $i=1$.

We define E(*one pair*) as the energy of the two-layered XY model with just one vortex pair of separation a in plane I. This vortex pair has been put in as a boundary condition on the θ variable in plane I. E(*no pair*) is the energy with novrotex pair in plane I. The energy for a vortex pair $E(a)$ is calculated as the difference between two thermodynamic expectation values of the energy $E(a) = E(\textit{one pair}) - E(\textit{no pair})$. In order to show that vortex fluctuations in the adjacent plane decouple the planes, we chose different sets of values for the Lagrangian multipliers.

For $\lambda^{\mathrm{I}} = 10$ and $\lambda^{\mathrm{II}} = 0$ we exclude vortex fluctuations in plane I, whereas there are no restrictions on plane II. A large λ^{I} is necessary in order to be able to study the two vortices in plane I at large separation. If we did not apply a Lagrangian multiplier to plane I, the following would happen. We induce (by the boundary condition) 1 + (vortex at position $\mathbf{x}_+$) and 1 − (vortex at position $\mathbf{x}_-$). As the separation between these two vortices is increased a − vortex will be created spontaneously close to the + vortex at position $\mathbf{x}_+$. Correspondingly, a + vortex will pop up next the position $\mathbf{x}_-$. We would then have two small vortex pairs at separation $a = |\mathbf{x}_+ - \mathbf{x}_-|$ instead of one pair of vortices at large separation a.

The energies measured for $\lambda^{\mathrm{I}} = 10$ and $\lambda^{\mathrm{II}} = 0$ are compared with the case where thermally activated vortices are excluded from both planes by choosing $\lambda^{\mathrm{I}} = \lambda^{\mathrm{II}} = 10$.

It is important to notice that the Lagrangian multipliers λ^ν only influence the vortex excitations and leaves the spin-wave spectrum unaffected. Moreover, we found no dependence of $E(a)$ on the value of $\lambda^\nu > 10$ as long as the Lagrangian multiplier is sufficiently strong to exclude the thermal activation of vortex pairs.

The bare vortex energies in Eq. (1) are calculated using the ordinary Metropolis algorithm.[8] We used a lattice consisting of two planes each of size 64×64. The values for the coupling constants are chosen as $J_\parallel = 1.0$ and $J_\perp = 0.1$. The temperature is measured in units of $J_\parallel$. Results for the ordinary 2D XY model ($J_\perp = 0$) are used as a comparison to the layered system. The 2D XY model undergoes a vortex unbinding transition[9] at the critical temperature $T_c \approx 0.9$.[10–12] Under the critical temperature the vortices are bound together in pairs and above T_c a mixture of bound vortices and free vortices coexist.

We now turn to a discussion of the measured vortex energies $E(a)$ which we compare with the functional form given in Eq. (1).

In Figs. 1(a)–1(c), we show results for $E(a)$ at low ($T=0.1$), intermediate ($T=0.9$), and high temperatures

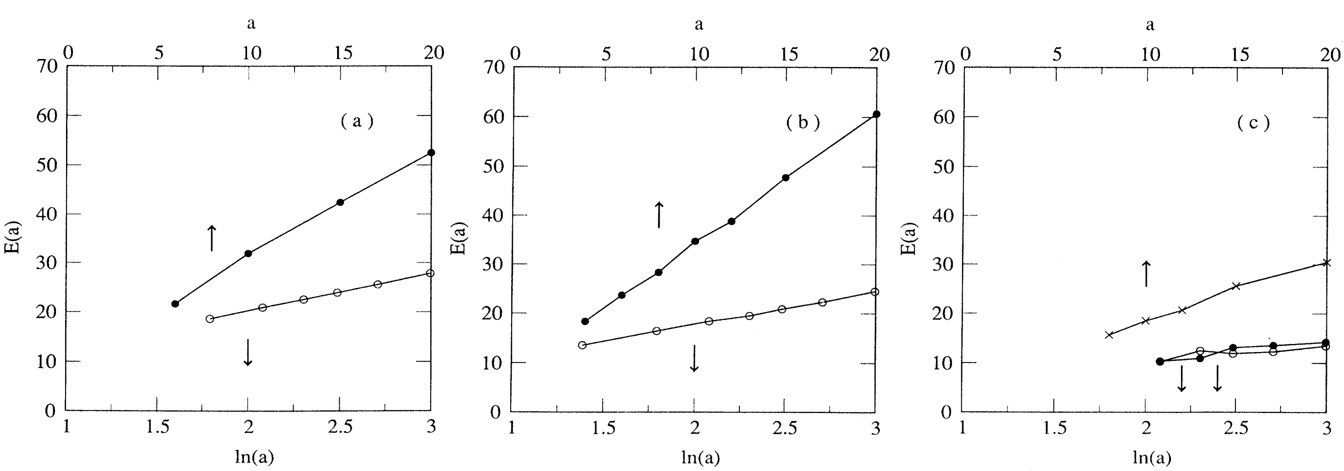

FIG. 1. Monte Carlo results for the energy $E(a)$ as a function of the vortex-pair separation for the layered system at three different temperatures: (a) $T=0.1$, (b) $T=0.9$, and (c) $T=1.8$. The energy is plotted either vs a (the x axis at the top of the figure) or vs $\ln(a)$ (the x axis at the bottom of the figure). The arrows on the graphs indicate which axis applies. In all three cases, $\lambda^{\mathrm{I}} = 10$ and $\lambda^{\mathrm{II}} = 0$. Solid circles represent the energy of the layered system. The open circles show the corresponding results for the 2D XY model. The crosses in (c) represent the energy for a layered system with no vortex fluctuations in either plane; here, $\lambda^{\mathrm{I}} = \lambda^{\mathrm{II}} = 10$ was chosen. Solid lines are only guides to the eye.

($T=1.8$). The energy of the layered system (solid circles) is plotted as function of a (the axis at the top); whereas for the 2D XY model (open circles), we plot the energy as function of $\ln(a)$. Unless indicated, λ^{II} in plane II is zero and in plane I, $\lambda^{I}=10$. At the low temperature considered in Fig. 1(a), only low-energy spin-wave excitations are present. Hence, we expect the form of the zero-temperature mean-field result in Eq. (1) to apply. This is supported by Fig. 1(a) since $E(a)$ is found to be linear in a (except at the shortest separations) when $J_\perp>0$. Notice that we recover the familiar logarithmic form of $E(a)$ when $J_\perp=0$, since $E(a)$ given by the open circles in Fig. 1(a) is linear in $\ln(a)$.

In Fig. 1(b) we show a typical result for the intermediate range of temperatures. For temperature $T=0.9$, coefficient E_1 of the 2D XY models jumps from a finite value to zero.[13] The important ingredient to renormalize E_1 to zero is the existence of thermally activated vortex pairs.[14,15] These pairs are suppressed here by the Lagrangian multipliers. Consequently, E_1 has not renormalized to zero for the results (open circles) shown concerning the 2D XY model. The solid circles are the results for the layered system. As can be seen, the interaction energy $E(a)$ is, even at this high temperature, dominated by the linear term predicted by the zero-temperature result in Eq. (1).

In Fig. 1(c) results for the temperature $T=1.8$ are shown. In this case, both the vortex energy measured for $J_\perp=0.1$ and $J_\perp=0$ are linear functions of $\ln(a)$. This is in clear contrast to the situation discussed above at lower temperatures. The vortex fluctuations in plane II have renormalized the coefficient of the linear term E_2 to zero. To stress the role of the vortex fluctuations we plot crosses on the same figure, where $E(a)$ measured with $\lambda^{I}=\lambda^{II}=10$ ensures that no thermally activated vortex pairs are present in either plane. This energy is linear in a. Our simulation shows that the reduction of E_2 from a finite value to zero occurs in a narrow temperature interval.

The vanishing of the linear term in Eq. (1) indicates that the planes become decoupled by the thermal fluctuations. To pursue the investigation of the effective coupling between the two planes, we divided the vortex-pair energy into contributions produced by the intraplane coupling plus the contributions from interplane coupling.

In Fig. 2 we show the energy for a fixed distance $E(a)$ ($a=15$) as a function of temperature. The total energy is given by the curve with the solid circles. The three other curves represent the following: the energy of plane I [the contributions from the first term in the Hamiltonian given by Eq. (2) and the second term in Eq. (3)] is given by the open circles, the asterisks show the Josephson contribution [second term in the Eq. (2)] of the energy, and the crosses indicate the energy in plane II. The energy $E(a)$ ($a=15$) is the sum of the three latter terms. The coefficient E_2 is a consequence of the Josephson coupling between the planes. Accordingly, we find that E_2 vanishes in the temperature region where the Josephson contribution to $E(a)$ ($a=15$) goes to zero. Below the temperature $T=1.3$ the functional form in Eq. (1) applies. Above the temperature $T=1.5$, the coefficient to the linear term E_2 vanishes and $E(a)$ assumes the ordinary logarithmic form.

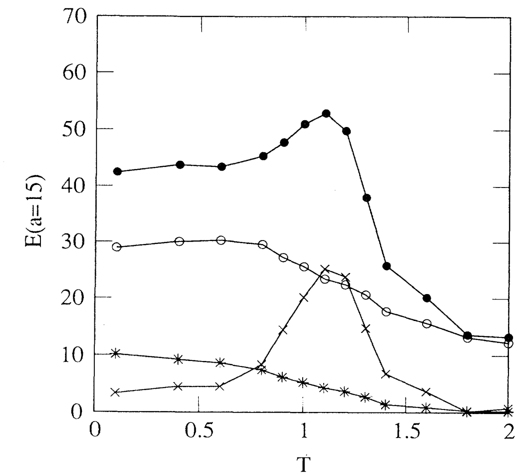

FIG. 2. Different contributions to the vortex-pair energy of a pair at fixed separation $a=15$. The value of the Lagrangian multipliers are $\lambda^{I}=10$ and $\lambda^{II}=0$. Solid circles represent the total energy of a vortex pair in plane I as a function of temperature. The other three curves represent the following: (open circle), the energy in plane I; (asterisks), the energy of the Josephson-coupling term; (crosses), the energy in plane II.

It is worthwhile pointing out that this temperature ($T=1.5$) is approximately the same as the transition temperature identified in the Monte Carlo study of the anisotropic 3D XY model by Chui and Giri in Ref. 16. In the study of the vortex-antivortex free energy in the anisotropic 3D XY model by Minnhagen and Olsson,[17] it is also concluded that the linear contribution to the free energy vanishes above a certain temperature. This temperature coincides with the temperature at which these authors find that the magnetization and the helicity modulus vanish.

Apparent from Fig. 2 is the peak in the energy of plane II (crosses). This indicates an increase in vortex number in plane II due to the existence of the pair in plane I. In Fig. 3 we show the excess in vortex number in plane II caused by the vortex pair in plane I. The extra vortices in plane II is a way for the system to release the strain in the Josephson energy between the two planes, caused by the existence of a vortex pair of separation a in plane I. Three curves are drawn for different separations of the vortex pair in plane I. The maximum number of vortices in plane II increases as the separation of the pair in plane I increases. However, the maximum number of induced vortices in plane II occurs at the same temperature for all three separations. Above this temperature the excess number of vortices rapidly vanishes. This indicates that, for all separation, the adjacent planes cease to be susceptible to each other with respect to vortex fluctuations as the temperatures is raised above a *specific* temperature $T^*\approx 1.5$ for the considered $J_\perp=0.1$. In this sense, the planes decouple for temperatures above T^*.

The thermal decoupling is also apparent from Fig. 4. In this figure we compare the number of *thermally* induced vortices $N_v(J_\perp=0)$ in the 2D XY model with the corresponding number $N_v(J_\perp>0)$ for the layered model. The difference $\Delta N_v=N_v(J_\perp>0)-N_v(J_\perp=0)$ is plotted as function of temperature. Both Lagrangian multipliers are

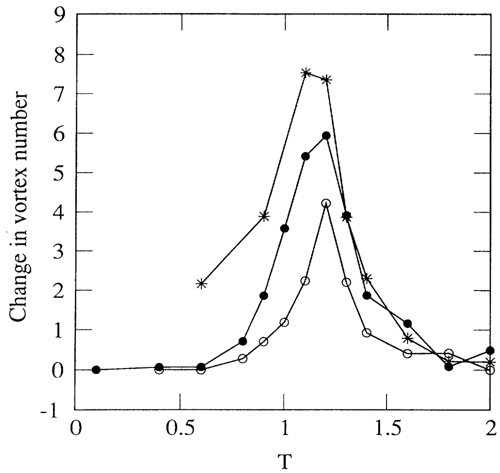

FIG. 3. The induced number of vortices in plane II caused by a vortex pair of fixed separation a in plane I as a function of temperature. The three curves represent different sizes of the vortex pair. Open circle, $a=10$; solid circles, $a=15$; and asterisks, $a=20$. The value of the Lagrangian multipliers are $\lambda^{\mathrm{I}}=10$ and $\lambda^{\mathrm{II}}=0$.

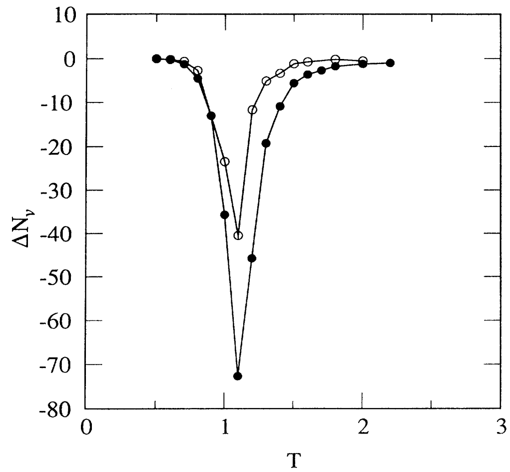

FIG. 4. The suppression of vortex fluctuations due to the Josephson coupling between planes in a $64\times64\times2$ XY model. The quantity ΔN_v is calculated as the difference $\Delta N_v=N_v(J_\perp\neq0)-N_v(J_\perp=0)$. Solid circles are for $J_\perp=0.1$ and open circles represent $J_\perp=0.05$. The value of the Lagrangian multipliers are $\lambda^{\mathrm{I}}=\lambda^{\mathrm{II}}=0$.

equal to zero and no vortex pair is imposed in plane I. The curve with open circles represents ΔN_v for $J_\perp=0.05$ and the solid circles $J_\perp=0.1$. Again a specific crossover temperature T^* can be identified. Below T^* the planes are highly susceptible to each other, as discussed above. ΔN_v is zero in this temperature region because both $N_v(J_\perp>0)$ and $N_v(J_\perp=0)$ are equal to zero. On the other hand, above T^* both $N_v(J_\perp>0)$ and $N_v(J_\perp=0)$ are nonzero but equal to each other. Hence, the thermally induced vortex density becomes the same for the layered system and for 2D XY model as soon as the temperature is increased above the decoupling temperature T^*.

We have studied the effect of thermal fluctuations on the bare vortex-antivortex interaction in a layered XY model. In particular, the role of thermally activated vortex fluctuations in the plane adjacent to the host plane of the considered vortex pair were investigated. These vortex fluctuations induce a crossover in the functional form of the vortex-pair energy $E(a)$ as function of separation a.

At low temperatures $E(a)$ depends linearly on a. A crossover in the behavior of $E(a)$ occurs in a narrow temperature region just above the vortex unbinding temperature of the 2D XY model. For temperatures above this region the usual 2D logarithmic dependence on vortex separation is retrieved despite the fact that $J_\perp>0$, i.e., the thermal fluctuations renormalize the effective interplane coupling to zero.

This finding might explain the fact that the 2D Coulomb-gas scaling theory describes the resistivity transition in the *layered* high-temperature superconductors at temperatures above the onset of resistivity, i.e., at temperatures above the vortex unbinding temperature.

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