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Vortex unbinding and layer decoupling in a quasi-two-dimensional superconductor

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The role of thermal vortices in the absence of applied magnetic fields is studied theoretically for anisotropic layered superconductors such as the high-T_c cuprates. Using a quasi-two-dimensional model and a real-space renormalization-group approach, the vortices are found to Josephson-decouple the superconducting layers slightly above T_c. The results are consistent with recent experiments and Monte Carlo simulations.

Dimensional crossover and other issues of dimensionality are of perpetual interest in statistical mechanics. The interplay between two-dimensional (2D) and three-dimensional (3D) physics has received special attention with the discovery of high-temperature superconductors (HTSC's). These materials are composed of stacked, coupled, 2D superconducting layers. Possible decoupling of these layers in the absence of an applied magnetic field has recently been demonstrated experimentally by Wan *et al.*,[1] and in computer simulations by Minnhagen and Olsson,[2] but is not yet understood theoretically.

In this article a quasi-2D model is studied in an attempt to resolve some of the fundamental dimensional aspects of the layered superconducting transition. The model is well suited to investigate the layer decoupling which may be triggered by interlayer phase fluctuations of the order parameter. Although the superconductors are considered here in the absence of any external field, the model also has important implications for finite magnetic fields. In zero field the fluctuations of interest are thermally excited neutral vortex pairs. In an applied field, $H > H_{c_1}$, vortices are induced with a temperature-dependent density which remains smaller than a maximum value of H/ϕ_0. As the transition temperature is approached from below, *thermal* vortex pairs begin to proliferate, thus playing a central role in the layered superconducting transition in low fields. It is shown below that layer decoupling can occur for anisotropic superconductors, and is mediated by thermal vortex pairs.

The high-temperature superconductors display a wide range of 2D and 3D thermodynamic and transport phenomena in the absence of an applied magnetic field. However, the theories employed to study particular aspects of the HTSC superconducting transition are not generally designed to address the full range of 2D and 3D behavior. For example, resistance measurements taken above the transition temperature[3] T_c show excellent agreement with predictions of flux flow theory[4] associated with the 2D vortex unbinding theory of Kosterlitz and Thouless[5] and Berezinskii[6] (KTB). Yet this theory predicts an absence of heat capacity anomalies, in conflict with recent observations.[7] The anomaly is commonly understood to require a 3D interpretation near the transition. Unfortunately 3D models cannot explain behavior such as the "universal jump" of the superfluid density,[4] observed in HTSC's through measurements of I-V characteristics.[3,8] A unified theory of 2D and 3D behavior could therefore serve as a useful foundation for existing theories in their interpretation of specific experimental situations.

Attempts to explain the observation of 2D behavior within 3D theory usually rely on the following line of reasoning: Due to the high anisotropy of HTSC's (quantified by the Ginzburg Landau anisotropy parameter $\gamma = \xi_{\parallel}/\xi_{\perp}$), the relevant *small* fluctuations of the order parameter are neutral vortex pairs which reside in the same layer. Only as fluctuations become larger than some length scale $r_{3\mathrm{D}}$ is it energetically favorable to form structures, such as vortex rings, which thread through multiple layers and eventually drive the transition.[9] The observation of this 3D behavior may be obstructed by finite size effects induced by the application of external probes. For the case of a current probe, vortex pairs which are normally bound below the transition are more easily dissociated by currents when the pair size is large. The saddle point[10] of the vortex-vortex interaction defines a probing length scale $r_I(I)$, which in turn describes a cutoff for scaling transformations such as the renormalization group (RG). Assuming $r_I < r_{3\mathrm{D}}$ leads to the conclusion that I-V characteristics probe the 2D nature of HTSC's.

A complete understanding of the zero-field transition must therefore have a 2D model as its starting point. However, the necessary inclusion of 3D fluctuations near the transition is not a straightforward procedure. Chattopadhyay and Shenoy have resolved this difficulty by adjoining a modified 2D KTB theory as input to an anisotropic 3D XY model.[9] In this picture, the layered system appears uniformly more isotropic upon renormalization, but it does not include the effects of fluctuations which eventually lead to layer decoupling.

Besides the Monte Carlo simulations mentioned above,[2] decoupling of layers has been investigated in other similar contexts for layered superconductors. It has been addressed theoretically in the mean field region[11] ($T \ll T_c$), in the region of strong fluctuations,[12] and as a result of fluctuations of the flux lattice.[13] Layer decoupling has also been discussed in terms of fluxon vortices which lie entirely between superconducting layers.[14,15]

Following previous theoretical approaches,[15–17] the zero-field layered problem is viewed here in terms of the Lawrence-Doniach model[18] (similar to the layered XY approach of Ref. 9) in which 2D Ginzburg-Landau layers are stacked and coupled via the Josephson mechanism. The logarithmic interactions of 2D vortices are modified by the Josephson coupling to become[19–21]

$$V(r) = 4\pi J\left[\ln\frac{r}{r_0} + \frac{1}{2}\left(\frac{r}{\lambda_J}\right)^2 \ln\frac{\lambda_J}{r}\right], \qquad r \ll \lambda_J. \quad (1)$$

Here, J is the in-plane coupling constant (proportional to the superfluid density), and r_0 is the vortex "diameter," representing the smallest scale of fluctuations. λ_J is the length scale associated with Josephson coupling and characterizes the decay of the gauge-invariant phase difference between layers due to fluctuations such as vortices. As discussed below, we are only interested here in the interactions between vortices of small separation.

Our effective Hamiltonian is written as

$$H = -\sum_{i\neq j} s_i s_j V(r_{ij}), \quad (2)$$

with the sum taken over all vortices i and j. We take $s_i = \pm 1$, according to the orientation of vortex i, and $\sum_i s_i = 0$. This form of the Hamiltonian assumes that interactions beyond two-body interactions may be ignored. While such an assumption has precedent,[16,17] there are other indications that three- and four-body terms also play an important role.[22] These latter arguments are not considered in the following analysis.

The fluctuations of a full multilayer system are modeled in terms of a 2D superconducting layer sandwiched between two superconducting slabs, as shown in the inset of Fig. 1(a). Thermal vortices are formed in the 2D layer (but not the slabs) and interact via $V(r)$, defined in Eq. (1). This geometry ensures that vortex fluctuations remain 2D. The picture is similar to that of a true multilayer superconductor at temperatures such that $\xi_\perp(T) < d$, with d the interlayer spacing. In this case fluctuations remain primarily 2D, and by definition are not expected to correlate between layers. It seems likely therefore that the effective Hamiltonian of Eq. (2), with Josephson interacting vortex excitations (JIVE's) defined through Eq. (1), will closely approximate the full multilayer system outside of the temperature regime near T_c. (Near T_c the characteristic fluctuation length scales are large and therefore of 3D nature.) A full multilayer analysis is required to test this assertion, and is not attempted here.

A phenomenological, real-space RG procedure is employed to investigate the transition in the model system.[23] Results are conventionally presented in terms of recursion relations for the renormalized coupling constants and the fugacity y. The fugacity is related to the energy $2E_c$, required to create a neutral pair of vortices of smallest separation through the expression $y = e^{-E_C/T}$. Adopting the KTB logarithmic scale $\ell = \ln r/r_0$ and the standard change of variables, $x = (T/\pi J) - 1$, gives recursion relations

$$\frac{dx}{d\ell} = (4\pi y)^2, \quad (3)$$

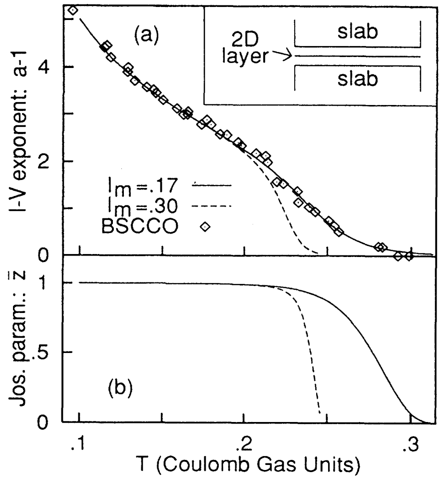

FIG. 1. (a) The I-V exponent, $a-1$, from $V \propto I^a$, is calculated using $a - 1 = 2/(1+x_m)$. x_m is the terminal value of x along a RG trajectory which has been truncated at length scale $\ell_m = 1.7$ (solid line) or $\ell_m = 3.0$ (dashed line) and is related to the partially renormalized superfluid density (Ref. 10). The parameter $\ell_m = 1.7$ is chosen to fit the displayed data points, taken from a single crystal of Bi-Sr-Ca-Cu-O (Refs. 8, 25). The horizontal axis is temperature in the Coulomb gas system (see Ref. 4). The inset shows the model system. (b) z_m is the terminal value of z along RG trajectories terminated as in (a) at $\ell_m = 1.7$ (solid line) or $\ell_m = 3.0$ (dashed line). z is the Josephson (inverse anisotropy) parameter, as described in the text. z_m is normalized as $\bar{z} = z_m/(z_0 e^{\ell_m})$ and drops strongly from one to zero, demonstrating effective layer decoupling. The horizontal axis is temperature in the Coulomb gas system.

$$\frac{dy}{d\ell} = \frac{2y\left[x + z^2(\frac{1}{2} + \ln z)\right]}{x+1}. \quad (4)$$

The dimensionless Josephson parameter z is defined as $z = r_0/\lambda_J$. These results are very similar to those found in Ref. 17 and Eq. (11) of Ref. 9, except that we assume here the interaction of Eq. (1) which is appropriate to pairs of small separation. The in-plane coupling J is weakened in the usual way by the polarization of small intervening pairs.[5] As expected, the recursion relations reduce to KTB as the Josephson coupling is turned off (i.e., when z is set to zero).

In the previously mentioned theories[9,16,17] it is correctly assumed that the Josephson parameter z (described above) must also be renormalized. By rescaling lengths, these authors arrive at a third recursion relation $dz = z\,d\ell$, which is solved as $z = z_0 e^{\ell}$, with $z_0 = r_0/\lambda_{J_0}$ being the *small* initial value of z associated with highly anisotropic materials (e.g., $z_0 \approx 0.5$ for Y-Ba-Cu-O, $z_0 \approx 0.04$ for Tl-Ba-Ca-Cu-O, and $z_0 \approx 0.03$ for Bi-Sr-Ca-Cu-O).

The exponential divergence of z at large scale ($z = z_0 e^{\ell}$), which is *independent* of temperature, is the result disputed here. It reflects only the apparent change in the interlayer spacing as lengths are rescaled. To determine whether decoupling is possible, the weakening of interlayer coupling due to fluctuations must also be included in the calculation. The details of this calculation are sketched below.

Current conservation in the 2D layer is expressed as $\nabla_{\parallel}^2\phi + 2\lambda_{J_0}^{-2}\sin\phi = 0$, where ϕ is the local phase difference between layers.[19] The response to a weak "probing" phase $\delta\phi$ in the presence of vortex-induced phase fluctuations ϕ_v is approximately $\nabla_{\parallel}^2\delta\phi + 2(\lambda_{J_0}^{-2}\overline{\cos\phi_v})\sin\delta\phi = 0$. Performing a spatial average $\overline{\cos\phi_v}$ and a statistical average over vortex configurations (denoted by brackets) gives the prescription, $\lambda_J^{-2} = \lambda_{J_0}^{-2}\langle\overline{\cos\phi_v}\rangle$, for inclusion of interlayer fluctuations. Similar prescriptions are applied in other analyses of layered superconductors.[11,13]

The spatial average $\overline{\cos\phi_v}$ for $\phi_v(\mathbf{r}', r)$ which describes the gauge-invariant phase difference between layers at location $\mathbf{r}'$ due to an isolated small pair of separation r is given as $\overline{\cos\phi_v} = (\pi L^2)^{-1}\int d^2r'\cos\phi_v \simeq 1 + (1/2)(r/L)^2\ln r/\lambda_J$, where πL^2 is the area of integration. The statistical average is performed using a RG technique in the spirit of Ref. 24, by which we integrate out configurations of the partition function which include vortex pairs of smallest separation. We define $C(r) = \langle\overline{\cos\phi_v}\rangle$ to include renormalization effects of all pairs smaller than r. The density of pairs whose size is in the range (r_0, r_0+dr) is[24] $dn = (2\pi r_0 dr)(y/r_0^2)^2$. The correction to $C(r_0)$ then becomes $dC = (\overline{\cos\phi_v} - 1)\pi L^2 dn$. Here $\overline{\cos\phi_v} - 1$ is the contribution to the average from a single small pair and $\pi L^2 dn$ is the number of pairs.

Changing variables from C to $z = r_0/\lambda_J$ and rescaling lengths gives $dz = z(d\ell + dC/2)$. The third recursion relation becomes

$$\frac{dz}{d\ell} = z + \frac{1}{2}(\pi y)^2 z\ln z. \tag{5}$$

Apparent in this equation are the length rescaling of λ_J [first term on the right-hand side (rhs)] and the renormalization due to fluctuations (second term).

Since λ_J is the screening response length associated with Josephson coupling, it is expected to *grow* in the presence of vortex pairs (ignoring length rescaling). To see this we note that the Josephson screening response amounts to an attempt by the superconductor to "expel" phase differences between layers. This is accomplished by the flowing of Josephson (and in-plane) currents. The response of the superconductor to large fluctuations is hampered by the presence of small JIVE pairs in their vicinity. The weakened response is manifested through an increased response length scale. This effect *competes* with the reduction of λ_J due to RG length rescaling, as observed in Eq. (5). As demonstrated numerically below, this competition leaves z to grow exponentially at low temperatures (the expected result in the absence of fluctuations), but drives z strongly to zero at temperatures slightly above T_c (signifying decoupling).

The recursion relations (3)–(5) are numerically integrated to give RG trajectories in x-y-z parameter space. $E_c = 0.74$ is used throughout this paper and has been chosen so that the I-V exponent a, described below, matches experimental data. This sets the starting points for the fugacity $y_0 = e^{-E_c/T}$. The unit of energy is $4\pi J$. The starting point $z_0 = 0.03$ (appropriate for Bi-Sr-Ca-Cu-O) is used. Temperatures are given in reference to the Coulomb gas (CG) system and may be scaled appropriately for 2D and 3D superconductors using Minnhagen's Ginzburg Landau Coulomb gas model.[25]

As discussed above, RG trajectories flowing into the 3D region are not accurately determined by recursion relations (3)–(5). The fixed point itself is in the 3D region and may not be studied. The 3D region here corresponds to $\lambda_J < r_0$ (or $z > 1$) where r_0, λ_J, and z are renormalized quantities. The region $y > 1$ is similarly unphysical in KTB problems due to associated high vortex densities.[4] Numerical results therefore must incorporate finite scale cutoffs. Here these cutoffs are interpreted in terms of finite system size, defect length scales, or probing lengths (described above). The choice of cutoff has a nontrivial effect on results, and must be carefully considered in a complete analysis. In this work two cutoffs $\ell = \ell_m$ are employed in the RG iteration: small ($\ell_m = 1.7$) and intermediate ($\ell_m = 3$). The smaller is chosen to fit experimental data in Fig. 1(a) which is described below. Both cutoffs allow the conditions $y, z < 1$ to be everywhere satisfied, and are therefore congruous with a 2D interpretation of results.

As a basic test of the theory we calculate the I-V exponent a, which is related to nonlinear current flow, through the equation $V \propto I^a$. Below T_c, a is determined according to the 2D theory:[10] $a - 1 = 2/(1 + x_m)$, where x_m is the terminal value of x along a given trajectory with length scale cutoff ℓ_m. Results are presented in Fig. 1(a). The core energy E_c and the cutoff $\ell_m = 1.7$ act as the two main fitting factors, and allow for satisfactory reproduction of the experimental features observed in Bi-Sr-Ca-Cu-O single crystals[8,25] as shown. A purely 2D KTB result with a similar cutoff is not pictured, since it gives a fit nearly identical to the 2D JIVE curve. Although the fitting parameters used here may not be justified due to the lack of a microscopic theory, the same qualitative features are nevertheless obtained over a wide range of parameters. This suggests that I-V characteristics are indeed probes of 2D phenomena in this system and may be interpreted through the quasi-2D theory.

Layer decoupling is demonstrated by plotting the z values z_m, obtained at the cutoff ℓ_m. As a result of the cutoff, z is merely peaked at low temperatures, rather than divergent, as shown in Fig. 1(b). z_m has been normalized here as $\bar{z} = z_m/(z_0 e^{\ell_m})$ to keep its peak value unity. An effective decoupling of layers occurs as evidenced by the rapid drop of $\bar{z}$ towards zero, even under the severe finite size restrictions of $\ell_m = 1.7$. These results show that decoupling is well underway before fluctuations become 3D. Layer decoupling at high temperatures is therefore a quasi-2D property of this system.

These results are entirely consistent with the simulations of Minnhagen and Olsson[2] who have observed signs of decoupling slightly above T_c. Additionally, Wan *et al.*[1] have measured a sequential resistive transition in Bi-Sr-Ca-Cu-O in which the high-temperature transition is thought to be associated with layer decoupling.[1] These measurements are also compatible with results found here, although further work is required to theoretically characterize the sequential transition.

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