Staggered Flux Vortices and the Superconducting Transition in the Layered Cuprates

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We propose an effective model for the superconducting transition in the high-T_c cuprates motivated by the SU(2) gauge theory approach. In addition to variations of the superconducting phase we allow for local admixture of staggered flux order. This leads to an unbinding transition of vortices with a staggered flux core that are energetically preferable to conventional vortices. Based on parameter estimates for the two-dimensional *t-J* model we argue that the staggered flux vortices provide a way to understand a phase with a moderate density of mobile vortices over a large temperature range above T_c that yet exhibits otherwise normal transport properties. This picture is consistent with the large Nernst signal observed in this region.

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The nature of the pseudogap phase of the (hole-) underdoped high-T_c cuprates is one of the central questions of correlated electron physics. A number of scenarios are successful in capturing certain aspects of the problem. Yet many theories face substantial difficulties when it comes to combining the large number of experimentally established anomalies of the underdoped state. A new challenge in this context has been set out recently by the Nernst effect measurements in underdoped samples [1]. In these experiments a thermal gradient is applied in the copper-oxide planes. In the presence of a small out-of-plane magnetic field, a voltage drop perpendicular to the magnetic field and thermal gradient is observed. This voltage is interpreted as the phase slip signal arising from vortices moving from hot to cold. Thus the Nernst effect reveals the existence of substantial superconducting (SC) short range correlations over a sizable region, starting significantly below the pseudogap temperature T^*, but extending up to temperatures high above the low T_cs of underdoped samples.

At first sight the observation of vortices above T_c fits well into a scenario [2] where SC phase fluctuations destroy the long range coherence, and short range pairing correlations survive up to much higher temperatures. In view of the small superfluid weight of underdoped systems it is conceivable that the SC transition is driven by a vortex unbinding similar to the XY transition, with T_c disappearing like the doping x for $x \to 0$. However a simple phase fluctuation scenario faces the following problem. The creation of a vortex comes at a price, as the SC order parameter goes to zero in the vortex core and condensation energy is lost. In disordered films of conventional superconductors, where a Berezinskii-Kosterlitz-Thouless (BKT) transition can be observed, the mean-field (MF) critical temperature and the vortex unbinding temperature are similar, and due to the mean free path ℓ entering the effective coherence length $\xi = \sqrt{\xi_0 \ell}$ (with $\xi_0 \sim v_F/\Delta$), the vortex core energy $\sim \xi^2 \Delta^2 / \varepsilon_F$ becomes small near T_c, as Δ decreases faster for $T \to T_c$ than ξ increases. Thus the loss of condensation energy is limited and the vortices can be cheap. In contrast with that the high-T_c cuprates are in the clean limit and for underdoped samples the gap magnitude remains large up to temperatures far above the SC transition. Hence the vortex core energy E_c for bringing the gap magnitude down to zero inside the vortex would normally be expected to be huge (ε_F in BCS theory and of order J in our case), and only exponentially few of these expensive vortices could be created above the small T_c in underdoped samples. Then we would expect that the transport properties of the pseudogap state resemble those of a flux-flow (FF) phase. Transport resembling the normal state occurs only at high temperatures $\sim E_c$ when the vortices proliferate and overlap. However this picture is inconsistent with experiments. These show that above a limited fluctuation regime close to T_c the in-plane transport looks rather normal and signs of FF conductivity do not extend far above T_c — contrary to the Nernst signal. Apparently the conductivity σ_n due to a significant number of quasiparticles dominates over the FF conductivity $\sigma_{\rm FF}$ in the total conductivity $\sigma = \sigma_n + \sigma_{\rm FF}$. Thus one has to explain two things: where the normal excitations come from and why the FF contribution is small. $\sigma_{\rm FF}$ can be estimated to be $\propto \eta/n_V$, where n_V is the density of vortices either forced in by a magnetic field in the mixed state or generated thermally above the BKT transition. η is the friction coefficient for the vortex motion. The FF conductivity is small if η is small and n_V is not. Here we show that our model produces a moderately large n_V even for underdoped samples with low T_c. We also present an approximate calculation that yields a finite density of normal excitations. We will not attempt to calculate η in this work. An effect that may reduce η is the observed [3] small low-energy density of states in the vortex cores. This translates into small dissipation due to vortex motion and thus small $\sigma_{\rm FF}$. Note that η cannot become arbitrarily small if we want σ_n to dominate the conductivity, as the quasiparticles responsible for σ_n will cause some dissipation. Thus a small FF contribution requires a moderately large n_V at temperatures above the limited fluctuation regime near T_c.

An extreme way to normal transport properties just above T_c is to make the vortices very dense, so that they overlap just above T_c. Then it is hard to understand why the vortex Nernst signal persists to temperatures so high above T_c. A theory considering purely Gaussian SC fluctuations [4] gave good agreement for the Nernst effect in overdoped and optimally doped samples. However the description of underdoped samples becomes problematic and an additional suppression of T_c had to be invoked.

Thus neither very few and expensive nor too many and too cheap vortices seem to match the experimental picture [5]. What is needed is a theory which produces a core energy of order T_c rather than J. In other words we need to decrease the core energy by placing in the vortex core another nonsuperconducting state that is nearby in energy. There are several proposals in the literature [6] for such a cheap vortex core, mainly emphasizing the vicinity of the d-wave superconductor to other ordered states. Here we study the possibility of a staggered flux (SF) state inside the vortex [7,8]. This scenario has the advantage that it emerges naturally from the SU(2) invariance, i.e., the Mott insulating nature of the undoped state. Note that the vicinity to the Mott state is also responsible for the small superfluid stiffness $\rho_s \sim x$.

The idea that vortices in the underdoped system have SF cores ties in with a more general picture of the pseudogap state. This is derived from the SU(2) gauge theory for the t-J model and views the pseudogap regime as a thermally disordered state, where the system fluctuates between various types of short range order corresponding to mean-field states that would all become identical at zero doping. The two most prominent correlations are d-wave superconductivity — determining the ground state as soon as the other fluctuations freeze out at low T — and SF correlations. The latter represent, in addition to phase fluctuations of the SC order parameter, the lowest lying fluctuations around the SC state with the largest spectral weight [9]. The scattering of quasiparticles with these SF fluctuations may be related to the partial loss of the quasiparticle peaks in the pseudogap state [10].

Some of the ideas presented here carry over to other types of cheap vortices. Indeed there are indications [11] for antiferromagnetic (AF) ordering at low T in the vortex cores of optimally doped Tl compounds, and it is quite likely that the vortex core may contain both SF and AF correlations [12]. The focus on SC and SF correlations is an attempt to concentrate on the main tendencies suggested from the SU(2) approach. The SF state has the advantage that it has a gap structure similar to the d-wave superconductor and naturally explains the gap in the core. Other correlations, such as AF tendencies, may be viewed as additional instabilities, which naturally coexist with the SF order for small x.

Recently Ivanov and Lee [13] calculated the energy differences between SF and d-wave SC states using the Gutzwiller projection technique. Together with the computed superfluid stiffness this provides an estimate for the energy of a SF vortex. In Ref. [13] the vortex core turns out to be very small, but on the other hand the core state, taken to be a pure SF state, is likely to be too high in energy, and a better core state will increase the size of the core again. Keeping in mind these uncertainties and for the lack of better parameters we use the numbers of Ref. [13] as input for a generalized XY model.

Let us begin with the SU(2) MF theory [9]. Here we are interested in low temperatures. Hence we assume that the bosons carrying the electronic charge are condensed. The Hamiltonian for the fermionic spin degrees of freedom $f_{i\uparrow}, f_{i\downarrow}$ on the lattice sites i reads

$$H_f = \frac{J}{2}\sum_{\langle ij\rangle}\begin{pmatrix} f_{i\uparrow} \\ f_{i\downarrow}^\dagger \end{pmatrix}^\dagger \begin{pmatrix} -\chi + W_{ij} & \Delta_{ij} \\ \Delta_{ij}^* & \chi + W_{ij} \end{pmatrix}\begin{pmatrix} f_{j\uparrow} \\ f_{j\downarrow}^\dagger \end{pmatrix}. \quad (1)$$

χ contains the hopping and the constraint field $a_{0,3}$. Next we allow for local admixtures of the SF amplitude in exchange for the SC pairing, described by an angle θ_i [9], and fluctuations of the SC phase, α_i. The SF amplitude on the bond ij is given by $W_{ij} = i\Delta_0(-1)^{i_x+j_y}\times \cos[(\theta_i + \theta_j)/2]$ and the pairing amplitude is $\Delta_{ij} = (-1)^{i_y+j_y}\Delta_0 \sin[(\theta_i+\theta_j)/2]\exp[i(\alpha_i+\alpha_j)/2]$. The pure superconductor has $\theta = \pi/2$, while the two degenerate SF states have $\theta = 0$ and $\theta = \pi$.

Now consider an effective Hamiltonian for α_i and θ_i,

$$H = \sum_{\langle ij\rangle}\rho_s(x,\theta_i,\theta_j)\cos(\alpha_i - \alpha_j) + \sum_{i\notin \mathrm{VP}} m_\theta \cos^2\theta_i + K\sum_{\langle ij\rangle}(\theta_i - \theta_j)^2 + \sum_{\mathrm{VP}} H_V. \quad (2)$$

The first term is the phase stiffness of the SC phase that depends on doping x and the local θ. The second term is a mass term for θ that takes into account the energy difference between SF and SC state outside the vortex plaquettes (VP). The third term is a gradient term for the θ variation. The last term is the vortex core energy, $H_V = \sum_{i\in\mathrm{VP}}(m_n \sin^6\bar{\theta} + m_\theta)$. The sum is over the four sites on each of the VP. Here Δ_{ij} is assumed to vanish and according to Eq. (1), θ now describes an interpolation between the SF state ($\theta = 0, \pi$) and the zero flux state ($\theta = \pi/2$) which is a Fermi liquid. As discussed earlier, the Fermi liquid core is expected to be costly and the energy costs of the SF state and the Fermi liquid state are m_θ and $m_\theta + m_n$, respectively. The specific θ dependence chosen for H_V comes from the MF theory for uniform θ, and $\bar{\theta}$ is the average θ_i over the four sites of the VP. Requiring that the vortex core area $4a^2$ equals the vortex size $\pi\xi^2$ of a pure SF vortex in the microscopic calculation in Ref. [13], we obtain that the lattice constant of Eq. (2) is slightly larger than the one of the underlying t-J model with a scale factor of $\sim$1.2. We assume that the variation of the vortex core size can be neglected at small x and low T.

In principle, (2) can be obtained from the MF theory as in Ref. [9] by integrating out the fermions and neglecting other collective modes with less spectral weight at low energies. Here however where possible we use parameters obtained by the Gutzwiller variational treatment of Ref. [13]. With $t/J = 3$, this gives $\rho_s(x, \theta = \pi/2) \approx 0.75xJ$, $m_\theta \approx 0.33xJ$, and $m_n \approx (0.25 - x)J/2$. The θ dependence of ρ_s is obtained numerically from MF theory which shows a rapid linear increase from zero when θ deviates from 0 or π. The coefficient K is difficult to extract from the collective mode spectrum [9], as the θ-mode is not simply quadratic around (π, π). Nevertheless its q dependence is weak and less than that of the SC phase α and vanishes for $x \to 0$. Thus we estimate $K \sim \rho_s/2$. Other choices give similar results.

In the scaling theory for the BKT transition [14] the vortex core energy is assumed to be large compared to the temperature such that the fugacity $y = \exp(-E_c/T)$ can be used as a small parameter. In the limit $y \to 0$ the transition occurs at $T_c = \pi\rho_s/2$. A nonzero fugacity $y > 0$ leads to a reduction of T_c from this upper bound by roughly $\pi^2\rho_s y$. With the parameters above the core energy of a single ideal SF vortex is $E_c = 0.75\pi xJ$ or twice the maximal $T_c^{\max} = \pi\rho_s/2$. This leads to a reduction of the critical temperature down to $T_c \approx 1.06\rho_s$.

The model described by Eq. (2) can be simulated with Monte Carlo methods. To estimate T_c we calculate the helicity modulus Υ which [15] measures the rigidity with respect to a phase gradient in the system. Υ vanishes above the SC transition: in BKT theory it jumps to zero at T_c, the height of the jump being $2T_c/\pi$, independent of the core energy [16]. We also measure the average θ variation inside and outside the vortex cores and how the number of vortices depends on doping and temperature.

A snapshot from the Monte Carlo is shown in Fig. 1 for a sample above T_c. We observe two relatively well isolated and other less separated vortices. The SC phase α_i is disordered but exhibits remnants of short range order. For $T = 0.09J$ and $x = 0.06$, θ varies rapidly in space due to its light mass $m_\theta < T$ and small gradient terms. Hence there is a significant amount of SF admixture reducing the SC pairing amplitude locally even outside the vortex cores (see shaded areas in Fig. 1). Outside the vortices, the average SF amplitude is $\langle|\cos\theta|\rangle \approx 0.3$ (compared to 1 for the pure SF state). Inside the vortex cores it is strongly enhanced, but not maximal ($\langle|\cos\theta|\rangle \approx 0.7$ for the sample shown, see also Fig. 3). In the left plot of Fig. 2 we show the helicity modulus Υ for two dopings x and a 100×100 system. Υ goes to zero above a doping-dependent temperature, but does not exhibit the universal jump of the XY model [15,16]. This is clearly a finite-size effect which is exacerbated by the small vortex density and which does not occur in the XY model where $E_c = 0$. An estimate for the true T_c is the intersection of the data with the line $2T/\pi$. This is based on the jump criterion $(\Delta\Upsilon)_{T_c} = \pi/2$ [16]. With that we arrive at $T_c^e \sim 0.75xJ \sim \rho_s$. A numerical bound is $T_c \leq xJ$. In a d-wave superconductor thermally excited nodal quasiparticles lead to an additional reduction of ρ_s that is not included here. We expect however that this does not affect the nature of the SC transition.

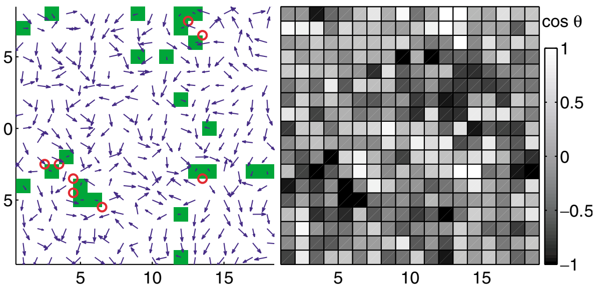

FIG. 1 (color online). Snapshot of the simulation for $x = 0.06$ and $T = 0.09J \approx 2T_c^e$. Left panel: Vortices (circles) and phase angles (arrows). The arrow length denotes the local SC amplitude. The shaded squares indicate sites with large SF admixture, $|\cos\theta_i| > 0.9$. The average value of $|\cos\theta|$ in the vortex cores is 0.7 (1 for the pure SF state). Right panel: $\cos\theta_i$.

The temperature and doping dependence of the vortex density n_V is summarized in the right plot of Fig. 2. The onset temperature for a finite n_V is an increasing function of x, approximately given by $T_V \sim \rho_s$. In the underdoped system there is a wider temperature range, starting at the BKT T_c and extending up to the mean field $T_c \sim 0.18J$ where n_V continues to increase and does not saturate. Thus the vortices do not overlap and there is the possibility that SC phase coherence is still well defined *locally* in a range above T_c. For $x = 0.06$ the phase correlation length ξ_α is $\sim$7 lattice spacings a at $T \sim 2T_c^e$. This is in contrast with the normal XY model where at $2T_c$, $\xi_\alpha \leq a$, and on average there is a vortex on every 5th site. We emphasize that in our model the phase fluctuations are not the only source of disorder. This can be seen in the right panel of Fig. 1. The SF fluctuations are not limited to the vortex cores and lead to sizable amplitude fluctuations as well. Thus the proximity to the Mott state gives rise to the low-energy scale for SF fluctuations and is responsible for

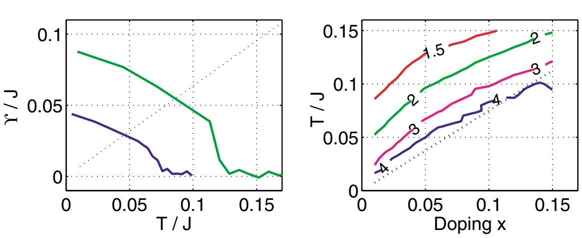

FIG. 2 (color online). Left panel: Helicity modulus Υ versus temperature T for dopings $x = 0.06$ and $x = 0.12$, averaged over 300 100×100 samples. The temperature where Υ goes to zero is an upper bound for the SC transition temperature T_c. The dashed line has the slope $2/\pi$. Right panel: Vortex density $\log_{10} n_V$ per site vs T and x. The dotted line is $T = \rho_s = 0.75xJ$.

both phase *and* amplitude fluctuations proliferating at comparable temperature scales.

We now address the electronic excitations. At finite doping the bulk SF state has small Fermi pockets. It is natural to expect that a state which fluctuates between a superconductor with gap nodes and a SF state will produce a finite density of states (DOS) at low energies. When we restrict the considerations to static configurations, we can calculate the quasiparticle spectrum of Eq. (1) on a finite system and average over many configurations of fluctuations. Results are shown in Fig. 3. The DOS exhibits a suppression for all T below the mean-field transition at $T \sim 0.18J$, but the gap fills in when T is increased through the SC transition. The local DOS is inhomogeneous, but is not simply correlated with or confined to the positions of vortices or regions of higher SF amplitude. These results share some aspects with a recent work by Eckl *et al.* [17] who considered disordering the d-wave superconductor by phase fluctuations. In their model the vortex cores are conventional and the core energy is zero by construction. Our generalized model accommodates both cheap vortices with SF core and energetically more expensive vortices with Fermi liquid core. Our calculation shows that already at the BKT T_c there is a finite number of quasiparticle excitations at low energies, and it is likely that the conductivity will be dominated by these normal excitations. The quasiparticle contribution to the Nernst signal however is small [1] and the vortex contribution will dominate at low T.

In conclusion, we have presented a simple model, motivated by the SU(2) approach for the high-T_c cuprates, that describes the superconducting transition as an unbinding transition of vortices with staggered flux core. Using parameter estimates from projected wave functions and the SU(2) mean-field theory it allows us to understand the occurrence of a moderate vortex density even for underdoped systems with low T_c. The vortex density is determined by an energy scale that is closely related to the energy difference between the SF and the d-wave SC state and that disappears towards zero doping, making the vortices relatively cheap. However there is a wider temperature range above T_c where the vortices are sufficiently dilute and do not overlap such that we expect that the superconducting phase coherence stays intact locally. This is in accordance with the interpretations of the Nernst effect measurements [1]. Phase and SF (i.e., amplitude) fluctuations lead to a filling in of the gap in the density of states at small energies already near the superconducting T_c. This could account for the normal-looking in-plane transport of the pseudogap phase which onsets just above the superconducting transition. A full analysis of this issue requires a calculation of the flux-flow resistivity in the fluctuating state. Although our approach involves rather strong simplifications and approximations we believe that it describes a way to understand the simultaneous occurrence of normal transport behavior (e.g., in the resistivity) and strong SC fluctuations, as witnessed by the vortex Nernst effect.

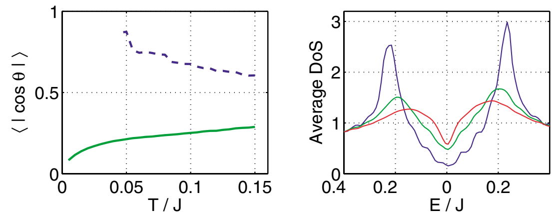

FIG. 3 (color online). Left panel: SF admixture inside (dashed line) and outside (solid line) the vortices vs temperature T for $x = 0.06$. Right panel: Density of states for $x = 0.06$ and $T = (0.01, 0.05, 0.13)J$, averaged over 25 samples (sizes 40×40 up to 48×48).

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