Nernst Effect and Diamagnetism in Phase Fluctuating Superconductors

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We study superconducting systems in the regime where superconductivity is destroyed by phase fluctuations. We find that the Nernst effect has a much sharper temperature decay than predicted by Gaussian fluctuations, with an onset temperature that tracks \( T_c \) rather than the pairing temperature. We find a close quantitative connection with diamagnetism—the ratio of magnetization to transverse thermoelectric conductivity reaches a fixed value at high temperatures. We interpret measurements on underdoped cuprates in terms of a dilute vortex liquid over a wide temperature range above \( T_c \).

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In recent years, the Nernst effect has emerged as an important probe of strongly correlated electron systems. The Nernst signal \( e_N \) is the electric field \( (E_x) \) response to a transverse temperature gradient \( \nabla T \) in the presence of a magnetic field \( H_z \), \( e_N = \frac{E_x}{\nabla T} \), with open circuit boundary conditions. A large-Nernst signal has been detected in the normal state of quasi-2\( d \) cuprate [1,2] and heavy fermion [3] samples and in thin amorphous films [4], well above \( T_c \). This is in contrast with typical (nonambipolar) metals, where the Nernst effect is usually weak: it was shown [5] that Fermi liquid quasiparticles with an energy-independent Hall angle do not contribute to \( e_N \) [5]. This, together with the proximity of the large-Nernst region to superconducting (SC) phases in some of these materials, points to fluctuating superconductivity as one natural source for the Nernst signal.

The Nernst signal can be expressed in terms of the electrical \( (\sigma) \) and thermoelectric \( (\alpha) \) conductivities as \( e_N = \frac{\sigma_x\sigma_y - \sigma_y\sigma_x}{\sigma_x^2 + \sigma_y^2} = \frac{\sigma_x}{\sigma_x} \). The second expression [6] is exact for systems with particle-hole symmetry, gives a good approximation to \( e_N \) for SC fluctuations, which lead to a large transverse thermoelectric response \( \alpha_{xy} \gg \alpha_{xx} \) [6,7]. Whereas fluctuations and quasiparticles both contribute to \( \sigma_{xx} \), fluctuations typically dominate \( \alpha_{xy} \). Thus, \( \alpha_{xy} \) is a more direct probe of fluctuations than \( e_N \).

Previous theoretical studies of the Nernst effect in fluctuating superconductors include the analysis of Gaussian fluctuations above the mean-field transition temperature [6] and a Ginzburg-Landau model with interactions between fluctuations of the order parameter [7]. These models give good agreement with experiments on thin amorphous samples [4] and with cuprate data in overdoped and optimally doped samples. For a 2\( d \) system, Gaussian fluctuations yield [6]

\[
\alpha_{xy}^{2d} = \frac{1}{3} \frac{e k_B}{\hbar} \frac{\xi^2(T)}{\xi_0^2} \approx \frac{H}{T - T_{MF}} 
\]

(1)

to linear order in field \( H \). Here, \( \xi(T) \) is the coherence length, \( \xi_0 \) the magnetic length, and \( T_{MF} \) the mean-field (MF) transition temperature. In the Gaussian regime, the magnetization for a 2\( d \) system is, to linear order in \( H \) [8],

\[
M_\zeta^{2d} = -2\frac{e k_B}{h} \frac{\xi^2(T)}{\xi_0^2} \]

(9). The ratio \( M_\zeta^{2d} \) is approximately constant in the Gaussian approximation even at high magnetic fields [6]. A connection between Nernst effect and diamagnetism was first seen in the experiments of Ref. [1]. However, whether such a connection is special to Gaussian fluctuations or a more general feature of SC fluctuations has not been established.

In this Letter, we study the Nernst effect and diamagnetic response due to thermal SC fluctuations in a phase-only model. Throughout, we assume that the order parameter \( \psi(x) = \Delta_0 e^{i\theta(x)} \) has frozen amplitude. This picture may describe the underdoped cuprates, where the pairing gap is thought to be much larger than \( T_c \) [10,11]. Here, phase coherence is lost via thermally generated vortex-antivortex pairs. Vortex diffusion has been proposed as the dominant contribution to the Nernst signal [1,12]. This picture is most useful in the dilute limit, when vortex spacing is much larger than the coherence length \( \xi_0 \) at \( T = 0 \). Then, vortices have a well-defined identity and the SC amplitude is suppressed only in the small area of the sample occupied by vortex cores.

Our starting point is the Lawrence-Doniach model of a layered superconductor, \( F_{LD} = - J_\perp \sum_{n} \sum_{i,j} \psi_{i,n}^* \psi_{j,n} e^{A_{ij}/2} \psi_{i,n} - J_\parallel \sum_{\langle n,m \rangle} \sum_{i} \psi_{i,n}^* \psi_{i,m} + U \sum_{n} \sum_{i} (\psi_{i,n}^2) + r/(2U)^2 \). Here, \( i, j \) label lattice points within a layer and \( n, m \) label the layers. The lattice vector potential due to an external magnetic field, \( A_{ij} = \frac{2}{h} \int_{i}^{j} \mathbf{r} \cdot \mathbf{A} \), is static and unscreened, corresponding to an extreme type-II superconductor. We consider the limit deep in the ordered phase within mean-field theory \( -r \gg k_B T \), where phase fluctuations dominate \( \psi_{i,n} = \Delta_0 e^{i\theta_{i,n}} \). This reduces the model above to an \( XY \) model. The interlayer coupling \( J_\perp \) stabilizes 3\( d \) superconductivity. However, we have verified that realistic val-
ues of $J_\perp$ increase $T_c$ relative to the $2d$ Kosterlitz-Thouless transition $T_{KT}$ only by a small amount. We have also verified that the normal state properties of interest are not significantly affected by $J_\perp$, except very close to $T_c$ or at low temperatures and high fields, where interlayer coupling leads to correlated vortex dynamics across different layers [7]. Hence, in what follows we set $J_\perp = 0$ and consider the $2d$ XY model with Josephson coupling $J = A_0^2 J$.

To study transport, we supplement this statistical mechanics model with model-A dynamics, describing coupling to a heat bath with no conservation laws [13]:

$$F_{XY} = -J \sum_{(ij)} \cos(\theta_i - \theta_j - A_{ij}),$$

$$\tau \dot{\theta}_i = -\frac{\partial F_{XY}}{\partial \theta_i} + \eta_i(t).$$

(2)

Here, $\tau$ provides a characteristic time scale for the dynamics. The stochastic noise $\eta$ is Gaussian correlated,

$$\langle \eta_i(t)\eta_j(t') \rangle = 2k_B T \delta_{ij} \delta(t - t').$$

(3)

These same dynamics are considered in studies of Gaussian fluctuations [6]. Our model corresponds to the strong coupling (frozen amplitude) limit of Ref. [7].

The model (2) and (3) has only three free parameters: $J$, $\tau$, and the lattice constant, $a$ [equivalent to a field scale, $H_0 = \Phi_0/(2\pi a^2)$, defined via the flux quantum $\Phi_0 = h c/2e$]. Of these, $J$ is an energy scale that fixes $T_{KT}$. The length scale $a$ is set by the average vortex separation at a temperature of order a few $T_{KT}$. It depends on the fundamental properties of vortices in the system in question, such as the vortex core energy [14]. In practice, $a$ is obtained by fitting the field dependence of $\alpha_{xy}$ and $M_z$ to experiment. Within $\xi_0$, the SC amplitude is significantly suppressed. Hence the dilute limit, where the vortex separation exceeds $\xi_0$, determines the $T$ window over which a phase-only description is appropriate. Finally, the time scale $\tau$ does not enter $\alpha_{xy}$, as can be shown from a Kubo formula involving the unequal time correlator $\langle j_i(t)\hat{j}_j(0) \rangle$, nor does it affect thermodynamic quantities, such as $M_z$. Hence, $\alpha_{xy}$ and $M_z$ in this model are only functions of $T/T_{KT}$ and $H/H_0$.

By an Onsager relation, $\alpha_{xy}$ can be obtained either from the electric current response to a $T$ gradient, $j_{T}\text{grad} = -\alpha_{xy} \nabla_T T$, or from the heat current response to an electric field, $j_{E}^0 = T \alpha_{xy} E_x$. A third method to compute $\alpha_{xy}$ is through the Kubo formula. As a check of our numerics and of the use of proper magnetization subtraction [15], we verified that all three methods agree for representative values of $H$ and $T$. We show results for the heat current response to an electric field $E$ (this method has the lowest statistical noise). We apply electric fields by making the vector potential in Eq. (2) time dependent and $T$ gradients by making $T$ in Eq. (3) position dependent. The electric and heat currents on the link from site $i$ to $j = i + \hat{a}$ are $j_{i\hat{a}} = J \sin(\theta_j - \theta_i + A_{ij})$ and $j_{i\hat{a}}^0 = -\frac{1}{2}(\partial \theta_i + \partial \theta_j)j_{i\hat{a}} + M^c (E \times \hat{z})$. These give the transport currents when summed over the sample. We use a cylindrical geometry (size ranging from $60 \times 60$ to $200 \times 200$) with free boundary conditions for the $\theta$s at the two edges of the cylinder. We obtain $M^c$ from the diamagnetic currents near the edges of the cylinder.

Intermediate $T$ regime.—Figures 1 and 2 show $\alpha_{xy}^{2d}$ on a single layer. Since $\alpha_{xy}^{2d}$ is independent of $T$, it only depends on the ratios $T/T_{KT}$ and $H/H_0$, and is expressed naturally in units of the $2d$ “quantum of thermoelectric conductance,” $2ek_B/h$. The inset of Fig. 1 shows $M_z$. Below $T_{KT}$, $M_z$ diverges logarithmically in $H$. The diamagnetic currents are due to a depletion of vortices near the sample edges, where the vortex density is smaller than the bulk density $H/\Phi_0$. The magnetization is analogous to the work function in a metal, and we find [16]

$$M_z^{2d} = \frac{2e \pi}{2h^2} \frac{T}{h} \log \frac{H_0}{H},$$

(4)

to leading order in $H$. This is similar to a previous result [17] and is in good agreement with our simulations.

High $T$ expansion.—For $T \gg J$, the phase-only model allows for an analytically tractable regime that is entirely different from the Gaussian regime. We expand in powers of $J/T$ using the Martin-Siggia-Rose formalism [16,18]. Since both $M_z$ and $\alpha_{xy}$ require a magnetic field, the expansion of these quantities involves graphs enclosing a finite flux. The leading term is given by the smallest closed graph—on a square lattice this involves 4 links and is hence proportional to $(J/T)^4$:

$$\alpha_{xy}^{2d} = \frac{2ek_B}{h} \frac{J}{2} \sin \frac{H}{H_0}. $$

(5)

FIG. 1 (color online). Transverse thermoelectric conductivity for a single plane. Inset: diamagnetic response.
of square (triangular) lattice. Despite the lattice dependence comparing to the Nernst signal $e_N$, fluctuations. It is surprising that a nonequilibrium property obtained in the Gaussian regime [6] extends to phase-only fluctuations, not considered in our simulations ($\times$ with error bars). Inset: log-log plot of $(\nu - \nu_B)\sigma_{ss}$ vs $T$. Data (●) and high $T$ expansion, Eq. (5), for $J_B$ (solid line) and $J_1$ (dotted line).
lattice, is $T^{-3}$). This strong decay, together with a more detailed quantitative comparison of experimental data on $\alpha_{xy}$ and $M_z$, would give strong evidence for phase fluctuations as the source of large-Nernst effect in the underdoped cuprates. The particular power law, $T^{-4}$, is consistent with our high-$T$ results on a square lattice. Given the $d$-wave symmetry of the cuprates, together with the fact that $a$ is a microscopic length, a few times the lattice spacing, the model could inherit the square symmetry of the underlying CuO$_2$ planes. However, it is difficult to establish from first principles whether these factors are sufficient to justify an effective square lattice model with only nearest-neighbor couplings.

The characteristic scale of $\alpha_{xy}$ at high $T$ is enhanced from what one would expect for a superconductor with $T_c = 28$ K. For example, the best fit to the square lattice high $T$ expansion requires $J = J_h = 52$ K, larger than the effective coupling $J_i = 30.2$ K that yields the correct $T_c$. This may be naturally attributed to thermal $d$-wave quasiparticles, omitted in this analysis. These suppress the long distance superfluid density [19] but not the superfluid density at shorter scales [16], which controls the high $T$ behavior. The ratio $J_h/J_i = 1.6$ is consistent with the $T$-dependent superfluid density in other cuprates [20]. A prediction from this scenario is that $M_z$ should continue to track $\alpha_{xy} T$.

\textbf{Onset.}—Wang et al. [1] define a temperature $T_{\text{onset}}$ where the fluctuating part of the Nernst effect can no longer be experimentally distinguished from the quasiparticle background. Here, since we have a natural scale for $\alpha_{xy}$, we define $T_{\text{onset}}$ as the temperature where $\alpha_{xy}^{2d}$ has decayed to a small fraction $\delta$ of the quantum of thermoelectric conductance, $\alpha_{xy}^{2d}(T_{\text{onset}}, H) = \frac{\alpha_{xy}}{\delta}$. For our model, $\alpha_{xy}^{2d} = \frac{2ek_b T^2}{h^2} F(T_{\text{onset}}, \frac{H}{T})$, hence, $T_{\text{onset}}$ is proportional to $T_c = T_{KT}$. The essential point is that, because $\alpha_{xy}^{2d}$ depends strongly on $T$, when inverted, $T_{\text{onset}}$ is only a weak function of $\delta$ and $H$. For instance, for the choice $H = H_0/4$ and $\delta = 0.01$ on the square lattice

$$T_{\text{onset}} = 3T_c. \quad (7)$$

This is consistent with the experimental observation that $T_{\text{onset}}$ roughly tracks $T_c$ as doping is varied [1]. Because of the strong $T$ dependence of $\alpha_{xy}$, the onset of Nernst effect is very sharp, in contrast to Gaussian fluctuations [6].

Measurements of $\sigma_{xx}$ do not have discernible fluctuating contributions at $T = T_{\text{onset}}$ [21]. This places an upper constraint on the parameter $\tau$, since $\sigma_{xx} \propto \tau$. The high $T$ expansion yields $\sigma_{xx}^{2d,\text{fluct}} = \frac{4e^2}{h} \frac{\pi f_{\text{fluct}}}{4} T^2$. As a benchmark, BCS theory predicts $\tau_{\text{BCS}} = 0.7h$. This yields a fluctuating conductivity at $T = 2T_c$ that is only $\approx 10\%$ of the quasiparticle conductivity in this material.

In conclusion, we studied the transverse thermoelectric conductivity $\alpha_{xy}$ and the diamagnetic response $M_z$ in the classical $XY$ model with Langevin dynamics. We obtain numerical results at low $T$ and analytic results at high $T$. We find the ratio $M_z/T \alpha_{xy}$ is an $O(1)$ number that depends only weakly on temperature and field—this, we believe, is a hallmark of SC fluctuations. For phase fluctuations, $\alpha_{xy}$ has a much more rapid $T$ decay (at least $\sim T^{-3}$) than for Gaussian fluctuations, where $\alpha_{xy} \sim 1/T$. Nernst measurements on underdoped LSCO display a sharp $T$ decay, in agreement with our model. We predict that $\alpha_{xy}$ and $M_z$ for different systems (e.g., different dopings) should collapse into a single curve when expressed in terms of the system-dependent $T_{KT}$ and characteristic field $H_0$.

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[9] To compare with experiments on thin film or layered samples, one must divide by the film thickness or layer separation $d$, $\alpha_{xy} = \alpha_{xy}^2/d$, and $M_z = M_z^2/d$.