Nernst Effect in Poor Conductors and in the Cuprate Superconductors

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(Received 16 January 2004; published 17 November 2004)

We calculate the Nernst signal in disordered conductors with the chemical potential near the mobility edge. The Nernst effect originates from the interference of itinerant and localized-carrier contributions to the thermomagnetic transport. It reveals a strong temperature and magnetic field dependence, which describes quantitatively the anomalous Nernst signal in high-T_c cuprates.

DOI: 10.1103/PhysRevLett.93.217002 PACS numbers: 74.25.Fy, 72.15.Jf, 74.40.+k, 74.72.–h

A significant fraction of research in the field of high-temperature superconductivity suggests that the superconducting transition is only a phase ordering while the superconducting order parameter remains nonzero above (resistive) T_c. This Letter describes how the unusual Nernst signal, which is one of the key experiments supporting that viewpoint, can be explained in a different manner as the normal-state phenomenon.

Thermomagnetic effects appear in conductors subjected to a longitudinal temperature gradient ∇T (in the x direction) and a perpendicular magnetic field $\mathbf{B}$ in the z direction. The transverse Nernst-Ettingshausen effect [1] (further the Nernst effect) is the appearance of a transverse electric field E_y in the third direction. The effect is known to be small in ordinary metals. Indeed in the framework of a single-band effective mass approximation with an energy dependent relaxation time $\tau(E)$, it appears only in the second order with respect to the degeneracy $k_B T/E_F \ll 1$ due to a so-called Sondheimer cancellation [2]. If τ is energy independent, the Nernst signal disappears even for nondegenerate carriers in the same approximation [3].

A sufficiently large positive Nernst effect was found in high-T_c cuprates in the vicinity of the resistive transition temperature T_c [4]. As in conventional superconductors it was attributed to the motion of vortices down the thermal gradient, while a small negative signal, measured well above T_c [5], was ascribed to the relaxation time decreasing with carrier energy. Such a negative signal may also originate from the counterflow of carriers with opposite sign (the familiar ambipolar Nernst effect), as explained by a simple two band model for electrons and holes with different mobilities [6], and/or from a charged density wave order [7], as observed in $NbSe_2$.

Recently, much attention has been paid to the anomalously enhanced *positive* Nernst signal observed *well above* T_c in $La_{2-x}Sr_{2-x}CuO_4$ (LSCO-x) in a wide range of doping x [8]. It has been attributed to the *vortex* motion, since the Sondheimer cancellation renders any "normal-state" scenario allegedly implausible [8]. As a result, the magnetic phase diagram of the cuprates has been revised with the upper critical field $H_{c2}(T)$ curve not ending at T_c. Most surprisingly, Ref. [9] reported H_{c2} as high as 40–150 T *at the zero-field transition temperature*, $T_c(0)$. Wang *et al.* [9] argued that the large Nernst signal supports a scenario [10] where the superconducting order parameter [i.e., the Bogoliubov-Gor'kov anomalous average $\mathcal{F}(\mathbf{r}, \mathbf{r}') = \langle \psi_\downarrow(\mathbf{r}) \psi_\uparrow(\mathbf{r}') \rangle$] does not disappear at T_c but at a much higher (pseudogap) temperature. Several other works [11,12] have also suggested that the anomalous Nernst effect is a result of $\mathcal{F}(\mathbf{r}, \mathbf{r}')$ fluctuations above T_c.

However, any phase fluctuation scenario is difficult to reconcile with the extremely sharp resistive and magnetic transitions at T_c in single crystals of cuprates. The uniform magnetic susceptibility at $T > T_c$ is paramagnetic, and the resistivity is perfectly "normal," showing only a few percent of positive or negative magnetoresistance. Both in-plane [13–15] and out-of-plane [16] resistive transitions remain sharp in the magnetic field in high quality samples providing a reliable determination of the genuine $H_{c2}(T)$. The vortex entropy estimated from the Nernst signal is an order of magnitude smaller than the difference between the entropy of the superconducting state and the extrapolated entropy of the normal-state obtained from specific heat [17]. These and a few other findings do not support any superconducting order parameter above T_c.

In this Letter we calculate the Nernst signal for a half-filled tight-binding band and for disordered conductors with the chemical potential, μ, close to the mobility edge. A brief review of the full range of experimental behaviors is given following the model. Unlike the half-filled band, Mott's law [18] for the variable-range-hopping conduction of localized carriers with any statistics and the Boltzmann kinetics for itinerant carriers yields the Nernst signal measured in a number of cuprates above the resistive $T_c(B)$. In underdoped cuprates, where preformed real-space pairs are expected [19], their Bose statistics and partial localization by disorder explain both the Nernst signal and a suppressed thermopower.

The Nernst voltage is expressed in terms of the kinetic coefficients σ_{ij} and α_{ij} as [3]

$$e_y(T,B) \equiv -\frac{E_y}{\nabla_x T} = \frac{\sigma_{xx}\alpha_{yx} - \sigma_{yx}\alpha_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2}, \tag{1}$$

where the current density per spin is given by $j_i = \sigma_{ij}E_j + \alpha_{ij}\nabla_j T$. Carriers in doped semiconductors and disordered metals occupy states localized by disorder and itinerant Bloch-like states. Both types of carriers contribute to transport if μ (or the Fermi level) is close to the mobility edge, where the lowest itinerant state appears. High-T_c cuprates are among such poor conductors, and their superconductivity appears as a result of doping, which inevitably creates disorder. Indeed, there is strong experimental evidence for the coexistence of itinerant and localized carriers in cuprates in a wide range of doping [19].

The standard Boltzmann equation in the relaxation time approximation yields for itinerant carriers

$$\sigma_{xx} = -e^2\sum_{\mathbf{k}} v_x^2 \tilde{\tau}(E_{\mathbf{k}})\frac{\partial f(E_{\mathbf{k}})}{\partial E_{\mathbf{k}}}, \tag{2}$$

$$\sigma_{yx} = -e^3 B\sum_{\mathbf{k}} \frac{v_x^2}{m_y}\tau(E_{\mathbf{k}})\tilde{\tau}(E_{\mathbf{k}})\frac{\partial f(E_{\mathbf{k}})}{\partial E_{\mathbf{k}}}, \tag{3}$$

$$\alpha_{xx} = -e\sum_{\mathbf{k}} \frac{E_{\mathbf{k}} - \mu}{T} v_x^2 \tilde{\tau}(E_{\mathbf{k}})\frac{\partial f(E_{\mathbf{k}})}{\partial E_{\mathbf{k}}}, \tag{4}$$

$$\alpha_{yx} = -e^2 B\sum_{\mathbf{k}} \frac{E_{\mathbf{k}} - \mu}{T}\frac{v_x^2}{m_y}\tau(E_{\mathbf{k}})\tilde{\tau}(E_{\mathbf{k}})\frac{\partial f(E_{\mathbf{k}})}{\partial E_{\mathbf{k}}}, \tag{5}$$

where $\mathbf{v} = \nabla_{\mathbf{k}} E_{\mathbf{k}}$ is the group velocity, $E_{\mathbf{k}}$ is the band dispersion, $1/m_i = \partial^2 E_{\mathbf{k}}/\partial k_i^2$ is the inverse mass tensor, which is assumed to be diagonal, $\hbar = c = 1$, $f(E_{\mathbf{k}})$ is the equilibrium distribution function, and

$$\tilde{\tau}(E_{\mathbf{k}}) = \frac{\tau(E_{\mathbf{k}})}{1 + [e\tau(E_{\mathbf{k}})B]^2/(m_x m_y)}. \tag{6}$$

Both α_{xx} and α_{xy} vanish at $T = 0$ for degenerate fermions with any $\tau(E_{\mathbf{k}})$, if their band is parabolic so that $1/m_i$ does not depend on $\mathbf{k}$. When τ does not depend on energy, two terms in the numerator of e_y, Eq. (1), cancel each other at any temperature in the parabolic approximation. However, a generalization of this Sondheimer cancellation for *any* band dispersion is flawed (see also Refs. [7,20]). The most striking example is a half-filled band. Modeling this band by the familiar tight-binding dispersion, $E_{\mathbf{k}} = -2t[\cos(k_x) + \cos(k_y)]$ yields $1/m_{x,y} = \cos(k_{x,y})/m$, where $m = 1/(2t)$, t is the nearest-neighbor hopping integral, and $\mu = 0$ for the half filling (we take the lattice constant $a = 1$). Then, by parity, $\sigma_{yx} = \alpha_{xx} = 0$, but α_{yx} is very large. Indeed calculating integrals, Eq. (2) and Eq. (5), we obtain at $k_B T \ll t$

$$e_y = -\frac{2t}{eT\Theta}\left(1 - 2\Theta \ln^{-1}\frac{1+\Theta}{|1-\Theta|}\right), \tag{7}$$

where $\Theta = eB\tau/m$. The Nernst signal is negative and superlinear, $e_y \approx -(2t/3eT)(\Theta + 4\Theta^3/15)$ at small $\Theta \ll 1$ with the minimum at $\Theta = 1$. It changes sign in a strong field, $\Theta > 1$, as shown in Fig. 1 (inset). In this simple example the number of electrons in the lower half of the band is equal to the number of holes in the upper half. As a result we arrive at a substantial *negative* Nernst voltage, Eq. (7), while both the thermopower, $S = -\alpha_{xx}/\sigma_{xx}$, and the Hall effect, $R_H = -B^{-1}\sigma_{yx}/(\sigma_{xx}^2 + \sigma_{yx}^2)$, equal zero at *any* temperature.

However, the half-filled band does not describe a range of behaviors of the Nernst signal and the thermopower (or $S\tan\Theta_H$) as observed in cuprates. In particular, Eq. (7) yields a wrong sign of $e_y \approx -60\ \mu$V/K and the magnitude, which is at least one order larger than observed with the typical values of $\Theta = 10^{-2}$ and $k_B T/t = 10^{-2}$ [4,8,9,17,21]. Moreover, unlike the half-filled band result, the Sondheimer cancellation, $S\tan\Theta_H \gg e_y$, holds in a wide temperature range, as shown in Fig. 1 for $YBa_2Cu_3O_{6.4}$. Here $S\tan\Theta_H = \sigma_{yx}\alpha_{xx}/(\sigma_{xx}^2 + \sigma_{xy}^2)$ represents the second term in Eq. (1); S and the Hall angle, $\Theta_H \approx \tan\Theta_H = BR_H/\rho$, were measured independently. As is clearly seen from Fig. 1, e_y and $S\tan\Theta_H$ are of the same order at sufficiently low temperatures, also in disagreement with the half-filled band results. Very similar trends of $S\tan\Theta_H$ and e_y were obtained for LSCO-0.2 with S, ρ, and R_H by Ref. [22]; in particular, e_y and $S\tan\Theta_H$ are of the same order near T_c. Besides, a noticeable suppression of the $S\tan\Theta_H/e_y$ ratio was reported to occur near T_c in some underdoped LSCO and Bi2201 at certain doping [8]. Below we discuss a realistic model with normal-state carriers (of any statistics) partially localized by disorder, which accounts for the unusual normal-state Nernst signal in cuprates.

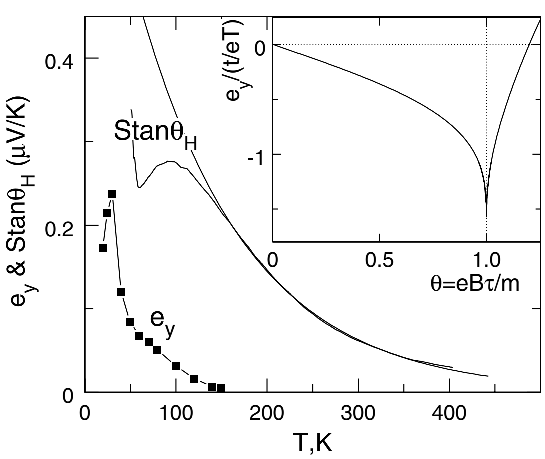

FIG. 1. The Nernst signal, e_y, and $Stan\Theta_H$ in $YBa_2Cu_3O_{6.4}$ at $B = 1$ T [21]. Inset: $e_y(B)$ in the half-filled band, Eq. (7).

When the chemical potential is near the mobility edge, the effective mass approximation can be applied. In this case, there is no Nernst signal from itinerant carriers alone, if τ is a constant. However, now the localized carriers contribute to the longitudinal transport, so that σ_{xx} and α_{xx} in Eq. (1) should be replaced by $\sigma_{xx} + \sigma_l$ and $\alpha_{xx} + \alpha_l$, respectively. Since the Hall mobility of localized carriers is often much smaller than their drift mobility [18], there is no need to add their contributions to the transverse kinetic coefficients. Neglecting the orbital effects ($\Theta \ll 1$ [8,9,21]), one obtains

$$e_y(T, B) = \frac{\sigma_l \alpha_{yx} - \sigma_{yx}\alpha_l}{(\sigma_{xx} + \sigma_l)^2}. \qquad (8)$$

When the chemical potential, μ, lies near the bottom of the band ($\mu \approx -4t$), α_{yx}, Eq. (5), and σ_{yx}, Eq. (3), are positive, but the thermopower of localized electrons with the energy below μ is negative, $\alpha_l < 0$. Hence, there is no further "cancellation" in the numerator of Eq. (8) in this electron-doping regime. When μ is near the top of the band ($\mu \approx 4t$), α_{yx} remains positive, but σ_{yx} is negative and α_l is positive, so that there is no cancellation in the hole-doping regime either. In the *superconducting* cuprates the conductivity of itinerant carriers σ_{xx} dominates over the conductivity σ_l of localized carriers, $\sigma_{xx} \gg \sigma_l$, which allows us to simplify Eq. (8) as

$$\frac{e_y}{\rho} = \frac{k_B}{e} r\theta\sigma_l, \qquad (9)$$

where $\rho = 1/[(2s + 1)\sigma_{xx}]$ is the resistivity, s is the carrier spin, and r is a constant,

$$\frac{r}{2s+1} = \frac{e|\alpha_l|}{k_B\sigma_l} + \frac{\int_0^\infty dEE(E-\mu)\partial f(E)/\partial E}{k_B T \int_0^\infty dEE\partial f(E)/\partial E}. \qquad (10)$$

Here μ is now taken with respect to the band edge. The ratio $e|\alpha_l|/k_B\sigma_l$ is a number of the order of 1. For example, $e|\alpha_l|/k_B\sigma_l \approx 2.4$, if $\mu = 0$ and the conductivity index $\nu = 1$ [23]. Calculating the integrals in Eq. (10) yields $r \approx 14.3$ for fermions, and $r \approx 2.4$ for bosons.

The Nernst signal, Eq. (9), is positive, and its maximum value $e_y^{\max} \approx (k_B/e)r\Theta$ is about 5–10 μV/K with $\Theta = 10^{-2}$ and $\sigma_l \approx \sigma_{xx}$, as observed [8,17]. Actually, the magnetic and temperature dependencies of the unusual Nernst effect in the overdoped LSCO are *quantitatively* described by Eq. (9), if σ_l obeys the Mott's law, $\sigma_l = \sigma_0 \exp[-(T_0/T)^x]$, where σ_0 is nearly constant. The exponent x depends on the type of localized wave functions and the variation of the density of states, N_l, below the mobility edge [18,24]. In two dimensions one has $x = 1/3$ and $T_0 \approx 8\alpha^2/(k_B N_l)$, where N_l is at the Fermi level.

If the magnetic field is strong enough [25], the radius of the "impurity" wave function α^{-1} is about the magnetic length, $\alpha \approx \sqrt{eB}$. If the relaxation time of itinerant carriers is due to the particle-particle collisions, the Hall angle depends on temperature as $\Theta \propto T^{-2}$, and the resistivity is linear, $\rho \propto T$, since the density of itinerant carriers is linear in temperature, both for fermionic or bosonic (e.g., bipolaronic) carriers [26]. Hence, the model explains the temperature dependence of the normal-state Hall angle and resistivity in cuprates at high temperatures. Finally, using Eq. (9) and Mott's law, the Nernst signal is given by

$$\frac{e_y}{B\rho} = a(T)\exp[-b(B/T)^{1/3}], \qquad (11)$$

where $a(T) \propto T^{-2}$ and $b = 2[e/(k_B N_l)]^{1/3}$ is a constant. Evidently, the phonon drag effect should be taken into account at sufficiently low temperatures in any realistic model. One can account for this effect by replacing $E_{\mathbf{k}}$ in Eqs. (4) and (5) by $E_{\mathbf{k}} + mv_s^2\tau_{\rm ph}/\tau_{e-{\rm ph}}$ [3]. Here v_s is the sound velocity, $\tau_{\rm ph} \propto T^{-4}$ is the phonon relaxation time due to the phonon-phonon scattering, and $\tau_{e-{\rm ph}}$ is the electron (hole) relaxation time caused by electron-phonon collisions. In two dimensions, $\tau_{e-{\rm ph}} \propto T^{-1}$ [27], so that $a(T)$ in Eq. (11) is enhanced by the drag effect as $a(T) \propto T^{-6}$. The theoretical field and temperature dependences of $e_y/(B\rho)$, Eq. (11), are in excellent quantitative agreement with the experiment, as shown in Fig. 2. Moreover, thereby obtained $a(T)$ follows closely T^{-6} as seen in the inset of Fig. 2. The density of impurity states $N_l = 8e/(b^3 k_B) \simeq 4 \times 10^{13}$ cm^{-2}(eV)$^{-1}$ corresponds to the number of impurities $N_{\rm im} \lesssim 10^{21}$ cm^{-3}, as it should be.

In agreement with the experiment [8,9,21], our model of thermal magnetotransport predicts anomalous Nernst signal in cuprates *only* within the doping interval, where superconductivity is observed. Indeed, since the chemical potential is well below the mobility edge in the nonsuperconducting underdoped cuprates, and it is deep inside the Bloch band in heavily doped samples, there is no "interference" of itinerant and localized-carrier contributions in these extreme regimes. If carriers are fermions, then $S \tan\Theta_H$ should be larger than or of the same order as

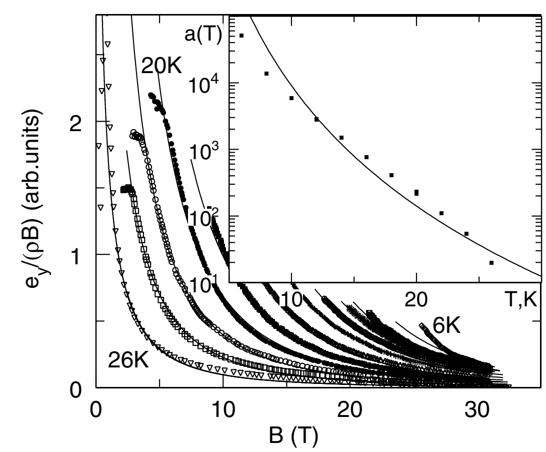

FIG. 2. Equation (11) fits the experimental signal (symbols) in LSCO-0.2 [9] with $b = 7.32$ (K/T)$^{1/3}$. Inset shows $a(T)$ obtained from the fit (dots) together with $a \propto T^{-6}$ (line).

e_y, because their ratio is proportional to $\sigma_{xx}/\sigma_l \gg 1$ in our model. To account for a low value of $S \tan\Theta_H$ in some underdoped cuprates, one should take into account that they are strongly correlated systems, so that a substantial part of carriers is (most probably) preformed bosonic pairs [19]. The second term in Eq. (10) vanishes for (quasi-)two-dimensional itinerant bosons, because the denominator diverges logarithmically. Hence, their contribution to the thermopower is logarithmically suppressed. It can be almost canceled by the opposite sign contribution of the localized carriers, even if $\sigma_{xx} \gg \sigma_l$. When it happens, the Nernst signal is given by $e_y = \rho\alpha_{xy}$, where $\alpha_{xy} \propto \tau^2$, Eq. (5). Different from that of fermions, the relaxation time of bosons is enhanced critically near the Bose-Einstein condensation temperature, $T_c(B)$, $\tau \propto [T - T_c(B)]^{-1/2}$, as in atomic Bose gases [28]. Providing $S \tan\Theta_H \ll e_y$, this critical enhancement of the relaxation time describes well the temperature dependence of e_y in Bi2201 and in strongly underdoped LSCO close to $T_c(B)$.

In conclusion, we calculated the Nernst signal in disordered conductors with the chemical potential near the mobility edge and found no ''Sondheimer cancellation'' of the signal. Sondheimer cancellation is also absent in the half-filled band, where the Hall effect and the thermopower are zero, but the Nernst signal is large and negative. Hence, a strong Nernst signal could arise from particular forms of the energy dispersion and the band filling. Unlike the half-filled tight-binding band, the model with itinerant and localized fermions and/or charged bosons describes quantitatively the anomalous Nernst effect in high-T_c cuprates as a normal-state phenomenon above the resistive phase transition. As far as the statistics of carriers is concerned, our boson or ''preformed pair'' picture is strongly supported by many other data in underdoped cuprates [19], while overdoped cuprates could be on the Fermi-liquid side. Unlike any fluctuating preformed pair scenario, e.g., [12], or ''preformed Cooper pair'' scenario [10], bosons in our model are perfectly normal and stable, so that there is no off-diagonal order [i.e., the *amplitude* of $\mathcal{F}(\mathbf{r}, \mathbf{r}')$ is zero] above their Bose-Einstein condensation temperature, T_c. There is no $\mathcal{F}(\mathbf{r}, \mathbf{r}')$ above T_c in the overdoped Fermi-liquid either. The localization of carriers by disorder is essential in any case. It is responsible for the strong magnetic field dependence of the Nernst signal, Fig. 2, or for the low thermopower in a few underdoped cuprates. Our results strongly support any microscopic theory of cuprates, which describes the state above the resistive and magnetic phase transition as perfectly normal, with $\mathcal{F}(\mathbf{r}, \mathbf{r}') = 0$. Unlike [9], our model does not require a radical revision of the magnetic phase diagram of cuprates [29].

This work was supported by the Leverhulme Trust (Grant No. F/00261/H). We would like to thank W. Y. Liang and K. K. Lee for helpful discussions.

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