Nernst effect in poor conductors and in the cuprate superconductors

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We calculate the Nernst signal in disordered conductors with the chemical potential near the mobility edge. The Nernst effect originates from interference of itinerant and localised-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.

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Thermomagnetic effects appear in conductors subjected to a longitudinal temperature gradient ∇T (in x direction) and a perpendicular magnetic field $\mathbf{B}$ in z direction. The transverse Nernst-Ettingshausen effect (further the Nernst effect) is the appearance of a transverse electric field E_y in the third direction. This effect as well as the longitudinal one were discovered by Nernst and Ettingshausen in a bismuth plate in 1886 [1]. The effect is known to be small in ordinary metals. Indeed in the framework of a single-band effective mass approximation it appears only in the second order with respect to the degeneracy $k_BT/E_F \ll 1$ due to a so-called Sondheimer cancellation [2], if the relaxation time $\tau(E)$ depends on energy. If τ does not depend on energy, the Nernst signal disappears even for nondegenerate carriers in the same approximation [3].

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 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 $La_{2-x}Sr_xCuO_4$ (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 but at a much higher temperature [9, 10]. Most surprisingly, Refs.[9, 10] estimated H_{c2} *at the superconducting transition temperature*, T_c, as high as 40-150 Tesla. Wang et al. [9] argued that the large Nernst signal supports a scenario [11], where the superconducting order parameter (i.e. the Bogoliubov- Gor'kov anomalous average $F(\mathbf{r},\mathbf{r}') = \langle\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}')\rangle$ does not disappear at T_c but at much higher (pseudogap) temperature T^*. Several other works [12] have also suggested that the anomalous Nernst effect is a result of the fluctuations of the superconducting order parameter 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 positive or negative magnetoresistance. Both in-plane [13, 14, 15, 16] and out-of-plane [17] 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 was found an order of magnitude smaller than the difference between the entropy of the superconducting state and the extrapolated entropy of the normal state obtained by specific heat measurements [18]. These and some other observations [19] do not support any superconducting order parameter above T_c.

In this Letter we calculate the Nernst signal for disordered conductors with the chemical potential, μ, close to the mobility edge. No 'Sondheimer cancellation' of the signal exists in this case. Mott's law [20] for the variable-range-hopping conduction of carriers localised below the mobility edge together with the Boltzmann kinetics for itinerant fermionic carriers or preformed bosonic pairs above the edge yields the Nernst signal, which agrees quantitatively with the signal in the superconducting cuprates at temperatures, $T > T_c(B)$ above the resistive phase transition.

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

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

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 localised by disorder and itinerant Bloch-like states. Both types of carriers contribute to the transport properties, if the chemical potential μ (or the Fermi level) is close to the energy, where the lowest itinerant state appears (i.e. to the mobility edge). Superconducting cuprates are among such poor conductors and their superconductivity appears as a result of doping, which inevitably creates disorder. Differently from 3D-conductors, the localised states cannot be 'screened' off by the itinerant carriers in these almost two-dimensional conductors even at high density of carriers. It is well known that in two dimensions a bound state exists for any attraction, however weak. Indeed, there is strong experimental evidence for the coexistence of itinerant and localised carriers in cuprates in a wide range of doping [21].

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

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

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

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

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

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

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

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 Ref. [7, 22]). The most striking example is a half-filled band. Modelling 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-neighbour hopping integral, and μ=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 $k_B T \ll t$

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

where $\Theta = eB\tau/m$. The Nernst signal is negative and super-linear, $e_y \approx -(2t/3eT)(\Theta + 4\Theta^3/15)$ at small $\Theta \ll 1$ with the minimum at Θ=1. It changes sign in a strong field, Θ>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 to a substantial *negative* Nernst voltage, Eq.(7), while both, the Hall effect, $R_H = -B^{-1}\sigma_{yx}/(\sigma_{xx}^2 + \sigma_{yx}^2)$ and the thermopower,

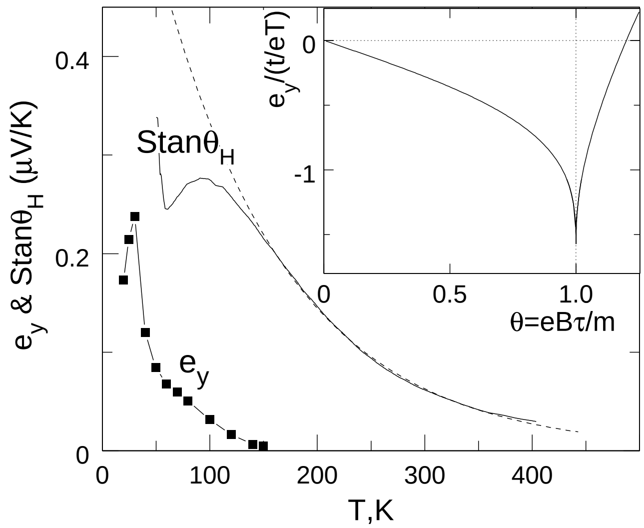

FIG. 1: The Nernst signal, e_y, and $S \tan\Theta_H$ in $YBa_2Cu_3O_{6.4}$ at B=1Tesla [10]. Inset: $e_y(B)$ in the half-filled band, Eq.(7).

$S = -\alpha_{xx}/\sigma_{xx}$, equal to zero at *any* temperature. Hence, the Sondheimer cancellation is an exception, rather than a rule. However, the thermomagnetic transport in the half-filled band, Fig.1 inset, does not describe the experimental results in cuprates. In particular, Eq.(7) yields a wrong sign of $e_y \approx -60$ μV/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, 10, 18]. Moreover, in disagreement with 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 it 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 e_y and $S \tan\Theta_H$ were obtained for overdoped LSCO-02 using independent measurements of S, ρ, and R_H [23], in particular, e_y and $S \tan\Theta_H$ are of the same order near T_c.

To account for these findings more realistic model is required. 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 localised 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 localised carriers is often much smaller than their drift mobility [20], there is no need to add their contributions to the transverse kinetic coefficients. Neglecting the orbital effects($\Theta \ll 1$ [8, 9, 10]) one obtains

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

When the chemical potential 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 localised 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 the chemical potential 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 localised carriers [21], $\sigma_{xx} \gg \sigma_l$, which allows us to simplify Eq.(8) as

$$\frac{e_y}{\rho} = \frac{k_B}{e} r\theta\sigma_l, \tag{9}$$

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

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

Here $N(E)$ is the density of states (DOS) near the band edge ($E = 0$), and μ is now taken with respect to the edge. The ratio $e|\alpha_l|/k_B\sigma_l$ is a number of the order of one. For example, $e|\alpha_l|/k_B\sigma_l \approx 2.4$, if $\mu = 0$ and the conductivity index $\nu = 1$ [24]. Calculating the integrals in Eq.(10) yields $r \approx 14.3$ for fermions ($s = 1/2$), and $r \approx 2.4$ for bosons ($s = 0$).

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, 18]. 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,

$$\sigma_l = \sigma_0 \exp\left[-(T_0/T)^x\right], \tag{11}$$

where σ_0 is about a constant. The exponent x depends on the type of localised wavefunctions and variation of DOS, N_l below the mobility edge [20, 25, 26]. In two dimensions one has $x = 1/3$ and $T_0 \approx 8\alpha^2/(k_BN_l)$, where N_l is at the Fermi level [27].

If the magnetic field is strong enough [28], 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 [29] or bosonic (e.g. bipolaronic) carriers [30]. 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 Eq.(11) the Nernst signal is given by

$$\frac{e_y}{B\rho} = a(T)\exp\left[-b(B/T)^{1/3}\right], \tag{12}$$

where $a(T) \propto T^{-2}$ and $b = 2[e/(k_BN_l)]^{1/3}$ 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 Eq.(4) and Eq.(5) by $E_{\mathbf{k}} + mv_s^2\tau_{ph}/\tau_{e-ph}$ [3]. Here v_s is the sound velocity, $\tau_{ph} \propto T^{-4}$ is the phonon relaxation time due to the phonon-phonon scattering, and τ_{e-ph} is the electron (hole) relaxation time caused by electron-phonon collisions. In two dimensions $\tau_{e-ph} \propto T^{-1}$ [31], so that $a(T)$ in Eq.(12) is enhanced by the drag effect as $a(T) \propto T^{-6}$. The theoretical field dependence of $e_y/(B\rho)$, Eq.(12), is in excellent quantitative agreement with the experiment, as shown in Fig.2 for $b = 7.32$ (K/Tesla)$^{1/3}$. The corresponding temperature dependence of $a(T)$ follows closely T^{-6}, inset to Fig.2. The density of impurity states $N_l = 8e/(b^3k_B)$ is about 0.4×10^{14} cm^{-2}(eV)$^{-1}$, which corresponds to the number of impurities $N_{im} \lesssim 10^{21}$ cm^{-3}, as it should be.

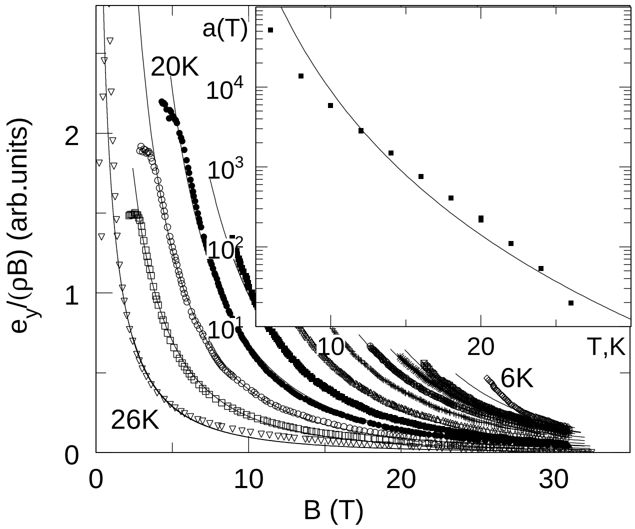

FIG. 2: Eq.(12) fits the experimental signal (symbols) in LSCO-02 [8] with $b = 7.32$ (K/Tesla)$^{1/3}$. Inset shows $a(T)$ obtained from the fit (dots) together with $a \propto T^{-6}$ (line).

In agreement with the experiment [8, 9, 10], our model of thermal magnetotransport predicts anomalous Nernst signal in cuprates *only* within the doping interval, where superconductivity is observed. Since the chemical potential is well below the mobility edge in the non-superconducting underdoped cuprates [21], and it is deep inside the Bloch band in heavily doped samples, there is no 'interference' of itinerant and localised-carrier contributions in these extreme regimes. If carriers are fermions, then $S\tan\Theta_H$ should be larger or of the same order as e_y, because their ratio is proportional to $\sigma_{xx}/\sigma_l \gg 1$ in our model. Although it is the case in many cuprates (eg., Fig.1, and the text below), a noticeable suppression of $S\tan\Theta_H$, as compared with e_y, was reported to occur close to T_c in strongly underdoped LSCO and in a number of Bi2201 crystals [8]. These observations could be generally understood if we take into account that underdoped cuprates are strongly correlated systems, so that a substantial part of carriers is (most probably) preformed bosonic pairs [32]. 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 cancelled by the opposite sign contribution of the localised 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). Differently 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 [33]. 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 $T_c(B)$. If some segments of a large Fermi-surface survive in underdoped cuprates, the Bose liquid of preformed pairs coexists with the fermionic carriers. The degenerate fermions virtually do not contribute to the thermal transport, but they dominate the longitudinal and transverse electric transport. Hence, the Hall coefficient and resistivity data could not present a behavior correlated with that of the Nernst signal.

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. In contrast with the half-filled band, the model with itinerant and localised fermions and/or charged bosons describe quantitatively the anomalous Nernst effect in high-T_c cuprates as a normal state phenomenon above the resistive phase transition. Our results strongly support any microscopic theory of cuprates, which describes the state above the resistive and magnetic phase transition as perfectly 'normal', $F(\mathbf{r}, \mathbf{r}') = 0$. Differently from [9, 10] the present model does not require a radical revision of the magnetic phase diagram of cuprates [34].

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