Nernst effect anisotropy as a sensitive probe of Fermi surface distortions from electron-nematic order

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We analyze the thermoelectric response in layered metals with spontaneously broken rotation symmetry. We identify the anisotropy of the quasiparticle Nernst signal as an extremely sensitive probe of Fermi surface distortions characteristic of the ordered state. This is due to a subtle interplay of different transport anisotropies which become additionally enhanced near van-Hove singularities.

Applied to recent experiments, our results reinforce the proposal that the underdoped cuprate superconductor YBa$_2$Cu$_3$O$_{6+\delta}$ displays such “electron-nematic” order in the pseudogap regime.

Spontaneous breaking of lattice rotation symmetry due to electronic correlations is currently in the focus of intense interest, most prominently in cuprate high-temperature superconductors such as YBa$_2$Cu$_3$O$_{6+\delta}$ (Refs. 1–3) and in the metamagnetic metal Sr$_3$Ru$_2$O$_7$ (Ref. 4). In analogy to liquid crystals, a phase with broken rotation (but preserved translation) symmetry has been dubbed electron nematic.$^5$

In cuprates, electron-nematic order has been discussed early on as intermediate phase which occurs upon melting of a uni-directional charge-density-wave (“stripe”) phase.$^{5-7}$ Microscopically, it is one of the known instabilities of the two-dimensional (2d) Hubbard model.$^{8-10}$ The first clear-cut signature of electron-nematic order in cuprates was found in neutron scattering experiments on YBa$_2$Cu$_3$O$_{6.45}$,$^1$ where the spin-fluctuation spectrum was found to develop a distinct anisotropic incommensurability below a temperature $T$ of about 150 K. Earlier transport measurements on YBa$_2$Cu$_3$O$_{6+\delta}$ (Ref. 11) also detected resistivity anisotropies $\rho_a/\rho_b$ of order 2 in the underdoped regime, but remained less conclusive.

The reason is that the crystal structure of YBa$_2$Cu$_3$O$_{6+\delta}$ contains CuO chains which break the otherwise tetragonal symmetry of the CuO$_2$ planes. In an order-parameter language, this implies a small field which couples linearly to the nematic order parameter. This has two main effects: (i) potentially existing nematic order will be aligned and (ii) a nematic ordering transition will be smeared out. While (i) enables observables to show a macroscopic anisotropy, which might otherwise be masked by domain formation, (ii) implies that electronic nematic order and purely structural effects cannot be sharply distinguished. Remarkably, locally broken rotation symmetry has been found on the surface of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ and Ca$_{2-x}$Na$_x$CuO$_2$Cl$_2$ using scanning tunneling microscopy.$^{12}$ In Sr$_3$Ru$_2$O$_7$, nematic order is a candidate explanation for the low-$T$ phase which masks the metamagnetic critical endpoint at around 8 T.$^4,13$ Resistivity anisotropies have been detected here, but a full picture has not yet emerged, because the rather unusual thermodynamics near the low-$T$ phase boundaries is not understood.

Very recent measurements$^2,3$ of the Nernst effect,$^{14}$ that is the transverse voltage induced by a thermal gradient in the presence of a magnetic field, have uncovered a surprisingly large anisotropy in YBa$_2$Cu$_3$O$_{6+\delta}$ below the pseudogap temperature. Consequently, this has been interpreted as evidence for broken rotation symmetry, but a theory which links this anisotropy to a particular ordered state was not available. Previously, the Nernst effect had been extensively studied as a probe of cuprate pseudogap physics,$^{15}$ but mainly interpreted as sign of precursor superconducting fluctuations. Only recently, a second contribution to the Nernst signal has been identified and associated to quasiparticle physics.$^{16}$ Theoretically, the quasiparticle Nernst effect in the presence of antiferromagnetic$^{17}$ and stripe$^{18}$ order has been investigated.

In this paper, we analyze, for the first time, the spatial anisotropy of the Nernst effect. We show that an enhanced and strongly anisotropic quasiparticle Nernst signal arises from the Fermi surface distortions which accompany broken rotation symmetry in metals. Surprisingly, small anisotropies in the kinetic energy can be easily enhanced by an order of magnitude in the Nernst signal, due the interplay of the anisotropies of conductivity and thermopower. A similarly large anisotropy does not arise from stripe phases. Hence, we establish the Nernst effect as a very sensitive and unique probe of electron-nematic order.$^{19}$ Applied to the measurements on underdoped YBa$_2$Cu$_3$O$_{6+\delta}$ (Refs. 2,3), we confirm the presence of the long-sought electron-nematic phase in the pseudogap regime.

Quasiparticle model. We shall calculate the thermoelectric response in a one-band model of quasiparticles. For concreteness, we work on a two-dimensional (2d) square lattice with a tight-binding dispersion

$$\varepsilon_k = -2t_1(\cos k_x + \cos k_y) - 4t_2 \cos k_x \cos k_y - 2t_3(\cos 2k_x + \cos 2k_y) - \mu.$$  \hspace{1cm} (1)

Such a 2d model is appropriate not only for cuprate superconductors, but (with some modifications) for a variety of other layered materials with tetragonal lattice structure, including Sr$_3$Ru$_2$O$_7$. To simplify calculations, we shall neglect inter-layer coupling, but will comment on its effect towards the end.

Nematic order distorts the band structure, which, on the mean-field level, can be captured by anisotropic hop-
Here we shall focus on the case of a $d_{x^2-y^2}$ electron nematic, as may arise from a Pomeranchuk instability in the $l = 2$ channel or as precursor of a stripe phase. We introduce an anisotropy parameter $\epsilon$, such that the hopping matrix elements obey $t_{1x,y} = (1 + \epsilon/2)t_1$ and $t_{3x,y} = (1 - \epsilon/2)t_3$. For $\epsilon \neq 0$, the lattice symmetry is thus broken from $C_4$ down to $C_2$.

**Transport theory.** The linear thermoelectric response is captured by three conductivity tensors $\sigma$, $\hat{\alpha}$, and $\hat{\kappa}$, which relate charge current $\vec{J}$ and heat current $\vec{Q}$ to electric field, $\vec{E}$ and thermal gradient, $\nabla T$ vectors:

$$\left( \begin{array}{c} \vec{J} \\ \vec{Q} \end{array} \right) = \left( \begin{array}{c} \hat{\sigma} \\ \hat{\kappa} \end{array} \right) \left( \begin{array}{c} \vec{E} \\ -\nabla T \end{array} \right).$$ (2)

The electrical field induced by a thermal gradient in the absence of an electrical current can be expressed by the linear response relation $\vec{E} = -\hat{\sigma} \nabla T$, and Eq. (2) together with $\vec{J} = 0$ yields $\vec{E} = \hat{\sigma}^{-1} \nabla T$. Therefore, the Nernst signal $\vartheta_{yx}$, defined as the transverse voltage $E_y$ generated by a thermal gradient $\nabla_x T$, reads

$$\vartheta_{yx} = -\frac{\sigma_{xx} \vartheta_{yx} - \sigma_{yx} \vartheta_{xx}}{\sigma_{xx} \sigma_{yy} - \sigma_{xy} \sigma_{yx}}$$ (3)

and $\vartheta_{xy}$ is obtained from $x \leftrightarrow y$. For a magnetic field $\vec{B} = B\hat{z}$ in $z$ direction, the Nernst coefficient is usually defined as $\nu_{yx} = \vartheta_{yx}/B$, which tends to become field-independent at small $B$. We employ a sign convention such that the vortex Nernst coefficient is always positive (formally $\nu_{yx} = -\vartheta_{yx}/B$, Ref. 20). In general, the Nernst coefficient can be negative or positive, for example if it is caused by the flow of charged quasiparticles.

The simplest description of quasiparticle transport is via the Boltzmann equation in the relaxation-time approximation. We assume a momentum and energy-independent relaxation time $\tau_0$, as appropriate for elastic impurity scattering at low temperatures. Then, the electrical and thermodiathermal conductivities read:

$$\alpha_{xx} = \frac{2e\tau_0}{T} \sum_k \frac{\partial f_k^0}{\partial \varepsilon(k)} \varepsilon(k) (v^z_k)^2,$$

$$\alpha_{xy} = \frac{2e^2 B\tau_0^2}{Thc} \sum_k \frac{\partial f_k^0}{\partial \varepsilon(k)} \varepsilon(k) v^y_k \left[ v^y_k \frac{\partial v^y_k}{\partial k_x} - v^x_k \frac{\partial v^x_k}{\partial k_y} \right],$$

$$\sigma_{xx} = -2e^2 \nu_{xy} = \frac{2e^2 B\tau_0^2}{Thc} \sum_k \frac{\partial f_k^0}{\partial \varepsilon(k)} \varepsilon(k) \left[ v^y_k \frac{\partial v^y_k}{\partial k_x} - v^x_k \frac{\partial v^x_k}{\partial k_y} \right],$$

where $\epsilon = |\epsilon|$ is the electron charge, $v_k$ the velocity, and $f^0_k$ the Fermi function. In this approximation, the Nernst signal is linear in both $T$ (at low $T$) and $\tau_0$. In the following, we shall be interested in the magnitude and anisotropy of the low-$T$ Nernst coefficient, i.e., we shall use Eqs. (4) to calculate $\nu_{xy}/T$ and $\nu_{yx}/T$.

**Numerical results.** We start with a survey of the Nernst signal in the $C_4$-symmetric case. $\nu/T$ is shown in Fig. 1a as function of the chemical potential and the second-neighbor hopping $t_2$, with $t_3$ kept zero. While $\nu/T$ is negative for all parameters, it is small for approximately circular-shaped Fermi surfaces, including the cases of small and large band filling for $|t_2/t_1| < 1/2$. (Note that $\nu/T$ remains non-zero in the limit of zero filling, as both the lattice effects and the Fermi energy vanish in this limit.) In contrast, the Nernst signal is large near the line $t_2 = \mu/4$ where the 2d van-Hove singularity is at the Fermi surface.

We now consider the sensitivity of the Nernst signal to a nematic distortion, i.e., a hopping anisotropy. Both $\nu_{xy}/T$ and $\nu_{yx}/T$ vary linearly with $\epsilon$, thus we plot the relative linear variation $(1/\nu)\partial(\nu_{yx} - \nu_{xy})/\partial \epsilon |_{\epsilon = 0}$ in Fig. 1b. As the Nernst signal itself, its variation is small for $\epsilon \approx 0.2 \ldots 0.4$ and $\mu/t_1 = -0.5 \ldots 0$, i.e., rather close to the van-Hove regime. We now discuss in more detail the thermoelectric response for such parameters. We choose $t_1 = 0.38$ eV and present results as function of hopping anisotropy for different (fixed) band fillings $n$ and different $t_2,3$. In YBa$_2$Cu$_3$O$_6+\delta$, the bare hopping anisotropy extracted from band-structure calculations is $|\epsilon| \approx 3 \ldots 4%$ with $t_a < t_b$ (i.e. $\epsilon < 0$ for $\hat{x}$ along the crystalline a axis) – this effect is primarily due to the coupling between planes and chains. Nematic order is expected to strongly amplify this anisotropy, and theoretical treatments have suggested anisotropies up to $|\epsilon| = 20\%$.

Fig. 2 shows the anisotropic elements of the response tensors $\sigma$ and $\hat{\alpha}$, together with the Nernst coefficient, for the crystal symmetry. Such a relation does not hold for $\alpha_{xy,\gamma x}$ in general, however, in the low-$T$ limit the Mott relation can be derived from Boltzmann theory, $\hat{\alpha} \propto \delta \sigma/d\mu$, implying that $\alpha_{xy} = -\alpha_{yx}$. Any anisotropy in the Nernst signal is therefore arising from $\sigma_{xx} - \sigma_{yx} \neq 0$ and $\alpha_{xx} - \alpha_{yx} \neq 0$ – both will have a piece which is linear in $\epsilon$. In general, the Nernst anisotropy at low $T$ will depend on the anisotropies of the Fermi surface, of the Fermi velocities, and of the scattering rate (the latter anisotropy is not taken into account in our calculation).

It is worth noting one limiting result: For the simplest anisotropic dispersive, $\varepsilon_k = (k_x^2/m_x + k_y^2/m_y)/2$ with $m_{yx,x} = (1 \pm \epsilon/2)m$, the anisotropies of $\sigma$ and $\alpha$ obtained in the Boltzmann framework (4) cancel in the Nernst signal, i.e., the Nernst signal remains zero due to Sondheimer cancellation. However, we shall obtain a large anisotropic Nernst response for non-parabolic dispersion.
FIG. 1: Evolution of the Nernst effect as function of chemical potential $\mu$ and second-neighbor hopping ($-t_2/t_1$). a) Nernst signal $\nu/T$ in the isotropic case, in units of $2.45 \times 10^3 V/(K^2 T) \times \tau_0/s$ for $t_1 = 1 eV$. b) Relative linear change of the Nernst signal with hopping anisotropy, $d(\nu_{xx} - \nu_{yy})/(\nu d\epsilon)$. In both panels, the white area corresponds to an empty band. For $-t_2/t_1 > 1/2$ the band minimum moves to $(0, \pi)$, $(\pi, 0)$. For $t_2 = \mu/4$ the van-Hove singularity is located at the Fermi level, where both the Nernst signal and its sensitivity to anisotropy are maximum. (Very close to this line the data are inaccurate due to discretization errors.) By particle-hole symmetry, the data for $t_2/t_1 > 0$ can be read off using $\mu \rightarrow -\mu$.

$t_2/t_1 = -0.4$, $t_3 = 0$ and band filling $n = 0.86$. While the anisotropy in the longitudinal conductivity $\sigma_{xx,yy}$ is moderate, Fig. 2a, there is a substantial anisotropy in $\sigma_{xx,yy}$, Fig. 2b. Remarkably, both anisotropies constructively interfere to generate a large Nernst anisotropy, Fig. 2c. The signal peaks at some finite $\epsilon$ where the Fermi-surface topology changes as a function of the anisotropy – this point again corresponds to a (now anisotropic) van-Hove singularity. Note that $\nu_{xy}$ can even change sign at some finite $\epsilon$, leading to a formal divergence of $\nu_{yx}/\nu_{xy}$. (Other additive contributions to $\nu$, e.g., from pairing fluctuations, may render this statement insignificant.)

A few remarks are in order. First, the thermopower $S = \sigma_{xx}/\sigma_{xx}$ comes out to be negative, Fig. 2b, also for $\epsilon = 0$. This is in contrast to the common wisdom that a single hole-like Fermi surface leads to a positive thermopower. Indeed, we obtain a positive (negative) thermopower in the limits of large (small) band filling, but the sign change in the $\mu-t_2$ plane is not tied to the topological change of the Fermi surface (i.e. the van-Hove singularity), but instead occurs above half filling for $t_2 < 0$. Second, the sign of the anisotropy in $\sigma$, Fig. 2a, is robust. This is physically transparent: $t_x > t_y$ implies a larger velocity along $\hat{x}$, and hence generically $\sigma_{xx} > \sigma_{yy}$. Third, the sign of the anisotropy ($\alpha_{xx} - \alpha_{yy}$), Fig. 2b, changes in the $\mu-t_2$ plane exactly at the van-Hove singularity. Notably, in Eq. (3) this sign change is compensated by the similar sign change of the Hall conductivity $\sigma_{xy}$, such that sign of the Nernst anisotropy is robust.

The influence of model parameters is illustrated in Fig. 3. For finite $t_3/t_2 < 0$, the van-Hove singularity is outside the regime of $\epsilon$ and $n$ which is relevant for cuprates. (This conclusion may be changed by bilayer splitting, see below and Ref. 10.) Fig. 3 also makes clear that the response of $\nu/T$ to moderate anisotropies is strongly non-linear near a van-Hove point.

**Discussion.** The large Nernst anisotropy for a nematic state prompts the question how this compares to other states with rotation symmetry breaking. For cuprates, the prime candidate is stripe order. Following Ref. 18, we have also calculated the Nernst anisotropy in various stripe states with real-space period 8 and 16. In most cases, the Nernst anisotropy for realistic parameter values is moderate, i.e., less than a factor of two. Exceptions are states with extremely elongated Fermi pockets, which we only encountered for period-4 charge-only stripes (and for which no evidence exists in YBa$_2$Cu$_3$O$_{6+\delta}$). Hence, stripe order is unlikely to explain the large Nernst anisotropy in YBa$_2$Cu$_3$O$_{6+\delta}$.
We thus confirm the interpretation of the data in Ref. 3, attributing the large anisotropy for 80 K < T < 150 K to a nematic state (while stripe-like order may set in at lower temperatures). Indeed, using $\epsilon = -0.2$ from Ref. 10, we can semi-quantitatively match the experimental results for YBa$_2$Cu$_3$O$_{6+\delta}$: We obtain a resistivity anisotropy $\sigma_y/\sigma_x \equiv \sigma_{yy}/\sigma_{xx} \approx 1.5$...2.5 (Ref. 11) and a Nernst anisotropy $\nu_y/\nu_x \equiv \nu_{yy}/\nu_{xx} \approx 4$...10 (Ref. 3).

Let us briefly discuss effects which were neglected in our calculation. A vertical dispersion from inter-layer coupling will smear the 2d van-Hove singularity, i.e., will different by a factor of order 5 – this we consider unlikely.

Conclusions. Our key result is a surprisingly large sensitivity of the Nernst anisotropy to symmetry-breaking Fermi-surface distortions, rendering the Nernst effect a unique tool to detect electron-nematic order. The effect is particularly strong for non-parabolic band dispersion, as occurs near van-Hove singularities and/or half-filling. We have provided a concrete theory for the measured Nernst anisotropies in YBa$_2$Cu$_3$O$_{6+\delta}$, pointing towards electron-nematic order in the pseudogap regime. We propose to search for Nernst anisotropies in other candidate compounds for such order, such as Sr$_2$RuO$_4$. Our results in Fig. 2 suggest that anisotropies of the thermopower are worth investigating as well.

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19. A probe which directly couples to the bulk quadrupolar order parameter of an electron-nematic phase is usually not available.
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21. This follows from the Kubo expressions for $\sigma_{xy,yx}$ or, for low $T$, from the geometric interpretation of the Hall conductivity, see: N. P. Ong, Phys. Rev. B 43, 193 (1991).
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