

Effects of Quasiparticle Ambipolarity on the Nernst Effect in Underdoped Cuprate Superconductors

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We consider the Nernst effect in the normal state of the underdoped cuprate superconductors, where recent quantum oscillation experiments have indicated the existence of Fermi surface pockets and quasiparticle ambipolarity in the excitation spectrum. Using an ambipolar d -density-wave model for the pseudogap, we predict a peak in the Nernst coefficient with decreasing temperature below the pseudogap temperature. The existence of the peak and its sign, which we predict to be the same as that due to mobile vortices in a superconductor, result from the dominance of the electron pocket at low temperatures, as has been observed in recent Hall experiments.

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The physics of the normal state of the cuprate high-temperature superconductors in the intermediate range of hole doping, called underdoping, is an important unresolved problem [1]. In this doping range, the system evinces a gap in the spectrum of unidentified origin (pseudogap) below a temperature scale $T^* > T_c$. An understanding of this pseudogap phase is widely believed to hold the key to the high transition temperature in the cuprates [1]. Encouragingly, recent quantum oscillation experiments [2–7] have found evidence of a remnant Fermi surface, consisting of small pockets, even in the enigmatic pseudogap phase. This has ushered in the encouraging prospect of describing this phase in terms of well defined low energy quasiparticles of a state with a broken symmetry and a reconstructed Fermi surface [3,8–10]. In this Letter, we will derive the implications of these important new ingredients in the cuprate physics on a widely discussed transport coefficient—the Nernst coefficient—using a well-known model of the pseudogap—the ambipolar d -density-wave (DDW) model [11,12]—which is consistent with the findings of the quantum oscillation experiments. It will be shown that the reconstructed Fermi surface and its low energy quasiparticles may help resolve another long-standing puzzle in the cuprate physics, that involving an enhanced Nernst signal at temperatures much above T_c [13–16]. An enhanced Nernst effect in the cuprates has been discussed before in terms of possible vortex motion in the pseudogap phase [17] and the superconducting fluctuation scenario [18]. While these approaches are expected to produce a large peak in the Nernst coefficient close to T_c , we show here that the quasiparticle ambipolarity associated with a competing ordered state can extend the onset temperature of a sizable Nernst signal to temperatures much higher than T_c .

The quantum oscillation experiments indicate that the Fermi surface in the underdoped cuprates is made of small pockets, giving rise to both hole- and electronlike charge

carriers (quasiparticle ambipolarity) in the excitation spectrum. Remarkably, the primary oscillation frequency is consistent with the existence of an electronlike pocket [19] in the excitation spectrum. This is despite the fact that the systems are actually moderately hole doped. A resolution of this puzzle may lie in the relative mobilities of the hole and the electronlike carriers: The oscillation frequency of the former may be strongly suppressed due to lower mobilities at low temperature (T) [3]. Even more convincing evidence that this may indeed be the case comes from the sign of the low- T , normal state Hall coefficient R_H [3,19]. In recent experiments [3,19] on yttrium barium copper oxide (YBCO), R_H has been observed to become negative for $T < T_0 < T^*$. This points to the dominance of the electron pocket at $T < T_0$ (T_0 : compensation temperature) over the closed holelike parts of the reconstructed Fermi surface. We will derive the implications of the ambipolar flow of the oppositely charged quasiparticles, and the low- T dominance of the electron pocket, on the Nernst coefficient using the ambipolar DDW model of the pseudogap as an illustrative example.

The ordered DDW model, as others [8–10], has enjoyed some success in explaining the quantum oscillation experiments in the pseudogap regime. Based on this illustrative model of quasiparticle ambipolarity, the principal result of this Letter is that the Nernst coefficient shows a pronounced peak with decreasing T in the pseudogap phase, as shown in Fig. 1. We also find that the sign of the low- T Nernst coefficient is the same as that due to vortices in a superconductor [20]. This sign is opposite to that above T^* and should be construed as a consequence of the low- T dominance of the electron pocket in the quasiparticle spectrum. The Nernst coefficient for the DDW state was studied earlier [21], but a pronounced low temperature peak with positive sign as discussed here was not found.

The commensurate DDW state [11] is described by an order parameter which is a particle-hole singlet in spin

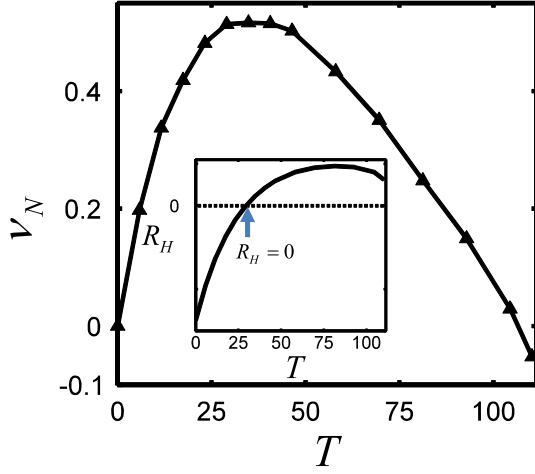


FIG. 1 (color online). Nernst coefficient ν_N in arbitrary units versus T in the ambipolar DDW state. The inset shows the Hall coefficient R_H calculated for the same set of ambipolar DDW parameters. Here $T^* = 110$ K, $A_e = 58$ K, $A_h = 253$ K, $t = 0.3$ eV, $t' = 0.3t$, $B_e = B_h = 1$, $W_0 = 0.1$ eV, and $\mu = -0.26$ eV, which corresponds to $x \sim 0.1$.

space:

$$\langle \hat{c}_{\mathbf{k}+\mathbf{Q},\alpha}^\dagger \hat{c}_{\mathbf{k},\beta} \rangle \propto iW_{\mathbf{k}} \delta_{\alpha\beta}, \quad W_{\mathbf{k}} = \frac{W_0}{2} (\cos k_x - \cos k_y). \quad (1)$$

Here \hat{c}^\dagger and \hat{c} are the electron creation and annihilation operators, respectively, on the square lattice of the copper atoms, $\mathbf{k} = (k_x, k_y)$ is the two-dimensional momentum, $\mathbf{Q} = (\pi, \pi)$ is the wave vector of the density wave, and α and β are the spin indices. In Eq. (1), $iW_{\mathbf{k}}$ is the DDW order parameter with the $id_{x^2-y^2}$ symmetry in the momentum space. For $\mathbf{Q} = (\pi, \pi)$, it is purely imaginary [11] and gives rise to spontaneous currents along the bonds of the square lattice.

The Hartree-Fock Hamiltonian describing the mean-field DDW state is given by

$$\hat{H} = \sum_{\mathbf{k} \in \text{RBZ}} \begin{pmatrix} \varepsilon_{\mathbf{k}} - \mu & iW_{\mathbf{k}} \\ -iW_{\mathbf{k}} & \varepsilon_{\mathbf{k}+\mathbf{Q}} - \mu \end{pmatrix}, \quad (2)$$

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y, \quad (3)$$

where $\varepsilon_{\mathbf{k}}$ is the band dispersion of the electrons and μ is the chemical potential. The Hamiltonian density in Eq. (2) operates on the two-component spinor $\hat{\Psi}_{\mathbf{k}} = (\hat{c}_{\mathbf{k}}, \hat{c}_{\mathbf{k}+\mathbf{Q}})$ defined on the reduced Brillouin zone (RBZ) described by $k_x \pm k_y = \pm\pi$ and can be expanded over the Pauli matrices $\hat{\tau}$ and the unity matrix \hat{I} : $\hat{H}_{\mathbf{k}} = w_0(\mathbf{k})\hat{I} + \mathbf{w}(\mathbf{k}) \cdot \hat{\tau}$, $w_0 = \frac{\varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{k}+\mathbf{Q}}}{2} - \mu$, $w_1 = 0$, $w_2 = -W_{\mathbf{k}}$, and $w_3 = \frac{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{Q}}}{2}$. The spectrum of the Hamiltonian consists of two branches with the eigenenergies $E_{\pm}(\mathbf{k}) = w_0(\mathbf{k}) \pm w(\mathbf{k})$, where $w(\mathbf{k}) = |\mathbf{w}(\mathbf{k})|$. For a generic set of parameters, corresponding to a nonzero hole doping in the underdoped regime of the cuprates, the reconstructed Fermi surface

consists of two hole pockets near the $(\pi/2, \pm\pi/2)$ points and one electron pocket near the $(\pi, 0)$ point in the reduced Brillouin zone. The existence of both hole- and electron-like excitations in the quasiparticle spectrum makes this state an ambipolar state.

In some recent Nernst experiments [13–15], a temperature gradient $-\nabla T$ is applied along the \hat{x} direction (T decreases along \hat{x}). For such a temperature gradient, and with a magnetic field \mathbf{B} along the \hat{z} direction, the vortices of a superconductor close to T_c produce a transverse electric field in the positive \hat{y} direction. With the sign convention that this signal is positive, the Nernst coefficient can be written as

$$\nu_N = \frac{E_y}{(-\nabla T)_x B} = \frac{\alpha_{xy} \sigma_{xx} - \alpha_{xx} \sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2}, \quad (4)$$

where σ_{ij} and α_{ij} are the electric and the thermoelectric conductivity tensors, respectively.

We calculate the off-diagonal element of the conductivity tensor σ_{xy} by using the solution of the semiclassical Boltzmann equation [22]:

$$\begin{aligned} \sigma_{xy}(\mu) = e^3 B \tau_e^2 \int \frac{d^2 k}{(2\pi)^2} & \left[\frac{\partial E_+(k)}{\partial k_x} \frac{\partial E_+(k)}{\partial k_y} \frac{\partial^2 E_+(k)}{\partial k_x \partial k_y} \right. \\ & \left. - \left(\frac{\partial E_+(k)}{\partial k_x} \right)^2 \frac{\partial^2 E_+(k)}{\partial k_y^2} \right] \left(- \frac{\partial f[E_+(k) - \mu]}{\partial E_+} \right) \\ & + (E_+ \rightarrow E_-; \tau_e \rightarrow \tau_h). \end{aligned} \quad (5)$$

Here the momentum integrals are over the reduced Brillouin zone. In the DDW band structure, the electron pocket near $(\pi, 0)$ is associated with the upper band $E_+(k)$. The first integral in Eq. (5), therefore, embodies the contribution to σ_{xy} due to the electronlike quasiparticles. The electron transport scattering time τ_e is taken as independent of the location on the electron Fermi line. The second integral in Eq. (5) with hole scattering time τ_h calculates the contribution to σ_{xy} from the hole pockets. In general, there is no obvious reason to expect $\tau_e = \tau_h$. For a consistent interpretation of the Hall effect experiments [3], it has been recently argued that the scattering times, which are directly proportional to the carrier mobilities, may in fact be different, and, at least at low T , $\tau_e > \tau_h$. With the above definition of the parameters, the diagonal element of the conductivity tensor is given by [22]

$$\begin{aligned} \sigma_{xx}(\mu) = e^2 \tau_e \int \frac{d^2 k}{(2\pi)^2} & \left(\frac{\partial E_+(k)}{\partial k_x} \right)^2 \left(- \frac{\partial f[E_+(k) - \mu]}{\partial E_+} \right) \\ & + (E_+ \rightarrow E_-; \tau_e \rightarrow \tau_h). \end{aligned} \quad (6)$$

From the solution of the Boltzmann equation at low T , the thermoelectric tensor α_{ij} is related to the conductivity tensor σ_{ij} by the Mott relation [23]: $\alpha_{ij} = -\frac{\pi^2}{3} \frac{k_B^2 T}{e} \frac{\partial \sigma_{ij}}{\partial \mu}$. Here $e > 0$ is the absolute magnitude of the charge of an electron. By using Eq. (4), the formula for the Nernst coefficient reduces to

$$\nu_N = -\frac{\pi^2}{3} \frac{k_B^2 T}{eB} \frac{\partial \Theta_H}{\partial \mu}. \quad (7)$$

Here $\Theta_H = \tan^{-1}(\frac{\sigma_{xy}}{\sigma_{xx}})$. Using Eqs. (5)–(7) and reasonable assumptions given below about τ_e and τ_h , we can calculate ν_N as a function of T in the ambipolar DDW state.

Recently, the normal state Hall coefficient $R_H = \frac{\sigma_{xy}}{(\sigma_{xx})^2}$ has been measured as a function of T in three different samples of underdoped YBCO [3]. In all three samples, R_H is positive above a temperature $T_0 < T^*$, which is consistent with the systems being moderately hole doped. Plots of R_H as a function of T reveal a change of sign from a positive R_H for $T > T_0$ to a negative R_H for $T < T_0$. By considering the possibility of the coexistence of electron and hole pockets in the normal state Fermi surface, it was shown before [24] that the flux flow mechanism in the mixed state of a superconductor ($H \ll H_{c2}$, $T < T_c$) can, in principle, produce a sign reversal of the Hall coefficient. Here, however, we do not focus on the flux flow mechanism, since the experiments [3] are carried out at much higher magnetic fields (~ 50 T), and, therefore, the drop in R_H below T^* ($> T_c$) and the subsequent change in sign are argued [3] to be unambiguously a property of the normal state. The drop of R_H below T^* can be explained naturally if the ordered state in question below T^* is inherently ambipolar, and the mobilities of the oppositely charged quasiparticles are assumed to be unequal and changing with T . For $\tau_e = \tau_h$, in which case the formula for R_H is independent of the scattering time, and for a generic set of parameters (t, t', W_0) consistent with the quantum oscillation experiments in YBCO [8,25], the size and curvature of the hole pockets are sufficiently bigger than those of the electron pocket. This implies that, for $\tau_e \sim \tau_h$, the sign of the overall R_H is positive [26]. We have checked that reasonable modifications of the band structure parameters cannot change this conclusion. Therefore, within Boltzmann theory, if at high temperatures ($T > T_0$) $\tau_e \sim \tau_h$, the Hall coefficient is positive. On the other hand, if $\tau_e > \tau_h$ for $T < T_0$, R_H can become negative at low T . Note that a higher mobility of the electronlike quasiparticles at low T is also consistent with the frequency observed in the quantum oscillation experiments [3,8]. An independent, microscopic, justification of the higher lifetime of the electronlike quasiparticles at low T and in the presence of a magnetic field follows by considering the scattering of both types of quasiparticles by vortices at low temperatures [27]. Because of the difference of the effective masses between the DDW quasiparticles near the antinodal and the nodal regions in the Brillouin zone, the electron lifetime due to vortex scattering can be significantly higher than the hole lifetime at low T in the presence of a magnetic field [25,28].

On the above grounds, we choose the minimal T dependence of the scattering times: $\tau_e^{-1} = A_e + B_e T$ and $\tau_h^{-1} = A_h + B_h T$. With these choices, we have calculated R_H for the ambipolar DDW state as a function of T with an

assumed mean-field T dependence of the order parameter: $W_0(T) = W_0 \sqrt{1 - (T/T^*)}$ ($T^* \sim 110$ K). We choose the values of the temperature-independent parameters A_e, B_e, A_h , and B_h by requiring that $\tau_e(T_0)$ is sufficiently larger than $\tau_h(T_0)$ for $R_H(T)$ to be zero at $T = T_0 \sim 30$ K and negative below this temperature. We have checked that our conclusions below for the qualitative behavior of ν with T are robust to any reasonable variation of the T dependence of τ_e, τ_h , and $W_0(T)$, as long as it supports the dominance of the electronlike quasiparticles at low T . Our results for R_H , with the above illustrative choice of the parameters, are plotted with T in the inset in Fig. 1.

We now use Eqs. (5)–(7), to calculate ν_N as a function of T for a specific value of hole doping $x \sim 10\%$. We use the value of x and the same set of parameters t, t' , and $W_0(T = 0)$ to calculate the value of μ , which determines the size and curvature of the hole and electron pockets. Using a mean-field T dependence of $W_0(T)$ and the phenomenological form of $\tau_e(T)$ and $\tau_h(T)$ above, we plot in Fig. 1 the calculated ν_N in the ambipolar DDW state as a function of T . Two important features of the qualitative behavior of ν_N with T are clearly visible in Fig. 1: First, ν_N has a pronounced peak at about $T \sim 35$ K, which is close, but not equal to, the compensation temperature $T_0 = 30$ K. The second important result, which is a consequence of the dominance of the electron pocket at low T , is that ν_N , at least near its peak, is of the same sign (positive) as the vortex signal near T_c . (The sign of ν_N is negative according to the older, textbook convention [29].) For both $T \sim T^*$ and $T \sim 0$, ν_N approaches zero, the former due to nearly perfect balance between the two types of quasiparticles [which can also make ν_N slightly negative, depending on the relative magnitudes of $\tau_e(T^*)$ and $\tau_h(T^*)$] and the latter due to the linearity of ν_N with T at low T [Eq. (7)], which is a remnant effect of the low- T Mott relation [23]. After restoring the \hbar and c , we estimate the peak value of ν_N in the pseudogap phase to be about 100 nV/KT, which is of the same order of magnitude as those observed in the experiments [13–16].

Because we have chosen two different scattering times for the holes and the electrons, it would be inconsistent to compare the value of ν_N in the ambipolar DDW state with that for $T > T^*$. However, we have checked that the quantity $\frac{\partial \Theta_H}{\partial \mu}$ in Eq. (7) is positive above T^* . Therefore, as T is decreased, somewhere near T^* the Nernst coefficient must change sign from negative to positive and show a peak as T is decreased further. The electron (hole) pocket gives a positive (negative) contribution to ν_N according to the sign convention used here. Since the electron pocket becomes dominant at low T due to the increase in mobility, ν_N is positive and rapidly increasing. However, at low enough T , it must approach zero, as shown in Eq. (7), which produces a pronounced low temperature peak. We have checked that these conclusions are valid irrespective of the specific choice of the T dependence of the scattering times, only as long as the mobility of the electronlike quasiparticles is

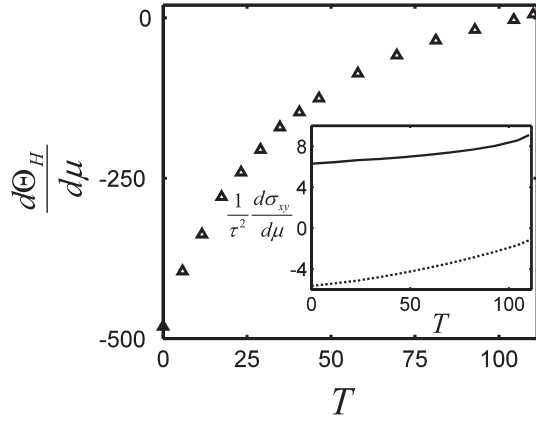


FIG. 2. Plot of the quantity $\frac{\partial \Theta_H}{\partial \mu}$ with T for the ambipolar DDW state. ν_N in Fig. 1 is derived from these values by multiplying with $-T$ in eV [Eq. (7)]. The inset shows the T dependence of $\frac{\partial \sigma_{xy}}{\partial \mu}$, which determines the T dependence of $\frac{\partial \Theta_H}{\partial \mu}$, separately for the hole (solid line) and the electron (dotted line) pockets.

sufficiently bigger than that of the holelike quasiparticles to produce a negative R_H at low T .

The origin of the sign of ν_N can be understood by plotting the quantity $\frac{\partial \Theta_H}{\partial \mu}$, which is proportional to ν_N [see Eq. (7)], as a function of T . This is shown in Fig. 2, where this quantity is negative in the ambipolar DDW state. Writing this quantity as $\frac{\partial \Theta_H}{\partial \mu} = \left(\frac{\partial \sigma_{xy}}{\partial \mu} \sigma_{xx} - \frac{\partial \sigma_{xx}}{\partial \mu} \sigma_{xy} \right) / (\sigma_{xx}^2 + \sigma_{xy}^2)$, we note that the second term in the numerator, which is proportional to R_H but turns out to be small, vanishes at T_0 . The T dependence of ν_N is mostly determined by the T dependence of $\frac{\partial \sigma_{xy}}{\partial \mu}$, whose values from the hole- and the electronlike pockets are given in the inset in Fig. 2. Since σ_{xy} depends sensitively on the curvature of the Fermi line in 2D, the values of $\frac{\partial \sigma_{xy}}{\partial \mu}$ from the individual pockets depend on how the corresponding curvatures change with small changes in the chemical potential. Since with an increase in μ the size and curvature of the electron pocket increases, the absolute magnitude of σ_{xy} from the electron pocket goes up as well. However, since the sign of σ_{xy} is itself negative from the electron pocket, $\frac{\partial \sigma_{xy}}{\partial \mu}$ is actually negative for the electron pocket as shown in Fig. 2. By similar reasoning we find that, with an increase in μ , the curvature of the hole pockets increases where the Fermi velocity is the largest, increasing the value of σ_{xy} . Therefore, $\frac{\partial \sigma_{xy}}{\partial \mu}$ is positive for the hole pockets. Since, with decreasing T , τ_e becomes larger in comparison to τ_h as indicated by the Hall experiments [3], the effects of the electronlike quasiparticles become dominant at low T , producing a rapid drop in $\frac{\partial \Theta_H}{\partial \mu}$ with T . This results in the rapid rise and positive sign of $\nu_N(T)$ with T . However, since at lower temperatures $\nu_N(T)$ is eventually linear in T [Eq. (7)] and, there-

fore, approaches zero, the Nernst coefficient in Fig. 1 has a peak, while $\frac{\partial \Theta_H}{\partial \mu}$ in Fig. 2 does not.

In conclusion, we show that a density-wave mediated Fermi surface reconstruction and quasiparticle ambipolarity in the underdoped regime of the cuprates imply a pronounced peak of the Nernst coefficient with decreasing temperature in the pseudogap phase. Within the ambipolar DDW model of the pseudogap, we find that the sign of the peak Nernst effect is the same as that expected from the vortices of a superconductor near T_c .

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