Violation of the isotropic-\( \ell \) approximation in overdoped \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \)

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Magnetotransport measurements on the overdoped cuprate \( \text{La}_{1.7}\text{Sr}_{0.3}\text{CuO}_4 \) are fitted using the Ong construction and band parameters inferred from angle-resolved photoemission. Within a band picture, the low temperature Hall data can only be fitted satisfactorily by invoking strong basal-plane anisotropy in the mean-free-path \( \ell \). This violation of the isotropic-\( \ell \) approximation supports a picture of dominant small-angle elastic scattering in cuprates due to out-of-plane substitutional disorder. We show that both band anisotropy and anisotropy in the elastic scattering channel strongly renormalize the Hall coefficient in overdoped \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) over a wide doping and temperature range.

The normal state transport properties of cuprates have proved as enigmatic as their high temperature superconductivity. One of the most striking properties to be uncovered is the anomalously strong temperature dependence of the Hall coefficient \( R_H \). This behavior is epitomized in \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) (LSCO), which spans the entire (hole-doped) phase diagram from the non-superconducting \( x = 0 \) to \( x > 0.34 \) [6, 7]. This is troublesome since at low temperature Hall data can only be fitted satisfactorily by invoking strong basal-plane anisotropy in the mean-free-path \( \ell \). This violation of the isotropic-\( \ell \) approximation supports a picture of dominant small-angle elastic scattering in cuprates due to out-of-plane substitutional disorder. We show that both band anisotropy and anisotropy in the elastic scattering channel strongly renormalize the Hall coefficient in overdoped \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) over a wide doping and temperature range.

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Within specific heat coefficient) is consistent with band structure (blue curve) (see Table I). The black dashed line represents the corresponding Fermi velocity whose peak value at $\varphi = \pi/4$ is $v_F(\varphi) = 4 \times 10^5$ m s$^{-1}$.

One important aspect of the FS topology shown in Fig. 1b (and not resolved in earlier measurements [8]) is the slight negative curvature as one moves from one apex of the diamond to another. This gives rise to alternating sectors on the FS that have electron- and hole-like character. Ong showed that for a 2D metal in the weak-field semiclassical limit, $\sigma_{xy}$ is determined by the ‘Stokes’ area $A = \int d\ell(k) \times \ell(k)$ swept out by $\ell(k)$ as $k$ moves around the FS. The local curvature of the FS gives rise to different ‘circulation’ of the $\ell$-vector and hence a contribution to $\sigma_{xy}$ with opposing sign. If, and only if, $\ell$ is significantly different on the different parts of the FS, can an overall sign-change in $\sigma_{xy}$ (and hence $R_H$) occur.

This effect is illustrated schematically in Fig. 2. The solid red line in Fig. 2a represents a 2D-projected FS with exaggerated negative curvature. The purple arrows indicate the direction and length of the $\ell$-vector for selected points on the FS. The angles between $\ell$ and $k$ and between $k$ and the $k_x$ axis are labelled $\gamma$ and $\varphi$ respectively. As $k$ moves along the FS away from the $k_x$ axis, $\varphi$ and $\gamma$ increase in the same sense. At a particular $k$-point, marked by $\star$, $\kappa = d\gamma/d\varphi$ changes sign and remains negative until $\varphi$ reaches $**$. At $\varphi = \pi/2$, $\gamma$ is once again equal to zero. If $\ell$ is anisotropic, as shown in Fig. 2b, loops of different circulation will appear in the $\ell_x$-$\ell_y$ plane. Ong demonstrated that $\sigma_{xy}$ will be determined by the sum of the areas enclosed by the primary (negative) and secondary (positive contribution to $\sigma_{xy}$) loops.

Let us now examine quantitatively the situation in LSCO30. The Fermi wave vector $k_F(\varphi)$ (blue curve in Fig.1b) and Fermi velocity ($v_F = \nabla_k \varepsilon_k$) (black dashed line in Fig.1b) are obtained from the tight-binding expression used by Yoshida et al. to map the FS underlying the quasiparticle peaks of their ARPES measurements on LSCO30 [10]: $\varepsilon(k) = E_0 = 2t(\cos k_x a + \cos k_y a) - 4t'(\cos k_x a)(\cos k_y a) - 2t''(\cos 2k_x a + \cos 2k_y a)$, where $t$, $t'$, and $t''$ are the first, second, and third nearest neighbor hopping integrals between Cu sites respectively. Note in Fig. 1b that the anisotropy in $v_F(\varphi)$ is large ($v_F(\pi/4)/v_F(0) = 3.5$) even at this elevated doping level.

To calculate $\rho_{ab}$, $R_H$ and $\Delta \rho_{ab}/\rho_{ab}$, we invert the conductivity tensor $\sigma_{ij}$ for a quasi-2D metal following Ref. [17] where $\sigma_{ij}$ is given in terms of $k_F(\varphi)$, $v_F(\varphi)$ and $\Gamma(\varphi)$. Assuming $\Gamma$ is isotropic at high $T$, one obtains $R_H(300) = -1.0 \times 10^{-10}$ m$^3$/C directly from the band parameters given in Table I more than 8 times smaller than the isotropic-$\ell$ limit. Thus, the ARPES-derived band anisotropy can account for almost all (> 90%) of the deviation of $R_H$ from the classical Drude result.

Encouraged, we proceed to consider other values of $x$. According to ARPES, $\epsilon_F$ crosses the van Hove singularity near $x \sim 0.18$, at which point, the FS becomes centered around $(\pi, \pi)$ [10]. As the FS approaches the saddle point, $t'/t$ increases (see Table I, the FS curvature is enhanced and the anisotropy in $v_F(\varphi)$ increases, implying even stronger renormalization of $R_H(300)$ with decreasing $x$. To illustrate this, we show in Fig. 3 the experimentally determined values of $R_H(300)$ for different $x \geq 0.18$ [3] together with $R_H$ calculated using just the band parameters extracted from ARPES (see Table I).

The experimental trend is well captured, both qualita-
absence of any experimental evidence for $T$-dependent FS reconstruction in LSCO, we deduce that this additional anisotropy must be contained in the elastic scattering rate $\Gamma_0(\varphi)$, presumably due to static impurities. According to AV, anisotropy in $\Gamma_0(\varphi)$ can arise from small-angle scattering off dopant impurities located between the CuO$_2$ planes \[12\]. If $d$ is the characteristic distance of such dopants from a plane, the electron scattering will involve only small momentum transfers $\delta k \leq d^{-1}$. Then, $\Gamma_0(\varphi)$ is proportional to $\delta k$ and the local density of states, i.e. to $1/v_F(\varphi)$. AV applied the same form of $\Gamma_0(\varphi)$ to the transport lifetime in order to interpret the $T$-dependence of the inverse Hall angle in cuprates within a marginal Fermi-liquid framework \[14\]. Although their derivation has subsequently been criticized \[22, 23, 24\], a predominance of forward impurity scattering in cuprates has been invoked to explain the weak suppression of $T_c$ with disorder \[25\], and the energy and $T$-dependence of the single-particle scattering rate $\Sigma''$ below $T_c$ \[26\].

In order to fit the transport data, we consider two functional forms of $\Gamma_0(\varphi)$: the AV form, $\Gamma_0(\varphi) = \beta/v_F(\varphi)$, and a squared sinusoid, $\Gamma_0(\varphi) = G_0(1 + \chi \cos^2(2\varphi))$, which makes $\Gamma_0$ less peaked at $\varphi = 0, \pi/2$. For LSCO30, $\rho_{ab}(T) = \rho_0 + AT^2$ below 50K \[13\]. We assume, as found in overdoped Tl$_2$Ba$_2$CuO$_{6+\delta}$ (Tl2201) \[27\], that the $T^2$ scattering rate is isotropic within the basal plane, i.e. it is the inelastic scattering that causes $R_H(T)$ to drop with increasing $T$. The intrinsic transport scattering rate can thus be written as $\Gamma(\varphi, T) = \Gamma_0(\varphi) + \alpha T^2$. For the AV fit, the parameters $\alpha = (1.6 \times 10^9 \text{ s}^{-1}\text{K}^2)$ and $\beta = (4.0 \times 10^{18} \text{ ms}^{-2})$ are constrained by $\rho_{ab}(T)$, implying there are no free parameters in the fitting of $R_H(T)$ and $\Delta_{\rho_{ab}}/\rho_{ab}(T)$. Note that this is not the case for the sinusoidal function. Finally a high-$T$ saturation component to the scattering rate (again parameter-free) is introduced, $\Gamma_{\text{max}} = (v_F/\alpha)$, consistent with the Ioffe-Regel limit ($\alpha$ being the lattice parameter \[17\] \[25\]). to take into account the deviation from $T^2$ resistivity above 50K and to ensure that $\Gamma$ eventually becomes isotropic. This leads to an effective scattering rate $\Gamma_{\text{eff}}(\varphi, T) = \Gamma^{-1}(\varphi, T) + \Gamma_{\text{max}}$ that is input into the calculation of $\sigma_{ij}$.

The experimental results and model outputs for $\rho_{ab}$, $R_H$ and $\Delta_{\rho_{ab}}/\rho_{ab}$ are compared in Fig. 3. All AV fits are in good quantitative agreement with the data at all $T$, despite there being no free parameters. The fit to $R_H(T)$ using the sinusoidal form of $\Gamma_0(\varphi)$ (dotted line in Fig. 4b) is equally good. (Here, $G_0 = 7.4 \times 10^{12} \text{ s}^{-1}$ and $\chi = 3.3$). However the same parameterization also leads to an overestimate of $\Delta_{\rho_{ab}}/\rho_{ab}$ by a factor of 6 at low $T$. Indeed, one cannot fit both $R_H$ and $\Delta_{\rho_{ab}}/\rho_{ab}$ satisfactorily using this form for $\Gamma_0(\varphi)$, despite the greater flexibility in the parameterization. This shortcoming demonstrates the sensitivity of the MR (a second-order process) to the form of the anisotropy in $\Gamma_0(\varphi)$ and suggests that the AV form is the more appropriate here. It is interesting to note that in La-doped Sr$_2$RuO$_4$, a very small

| $x$ | $t$ (eV) | $\xi_0/t$ | $-t'/t$ | $-t''/t'$ |
|-----|---------|----------|----------|----------|
| 0.30 | 0.25    | 0.990    | 0.120    | 0.5      |
| 0.28 | 0.25    | 0.960    | 0.121    | 0.5      |
| 0.25 | 0.25    | 0.918    | 0.125    | 0.5      |
| 0.22 | 0.25    | 0.880    | 0.130    | 0.5      |
| 0.18 | 0.25    | 0.837    | 0.140    | 0.5      |

**TABLE I**: Tight-binding band parameters for LSCO ($0.18 \leq x \leq 0.3$) interpolated from values given in \[10\].
amount of off-plane Sr-site substitution (∼1%) induces a sign change in $R_H(0)$ even though the FS topology, as revealed by quantum oscillations, is unchanged [29]. Just as in LSCO, Sr$_3$RuO$_4$ contains both electron- and hole-like regions of FS. This supports our conjecture that it is anisotropy in $\Gamma_0(\varphi)$, rather than FS reconstruction, that causes $R_H(T)$ in LSCO to grow with decreasing $T$.

Finally, we note that in Tl2201, the isotropic-ℓ approximation appears to hold at low $T$ [27, 30], even in the presence of significant out-of-plane disorder (both interstitial oxygen and Cu substitution on the Tl site). The key difference here is perhaps the band anisotropy. According to ARPES [31], $v_f(\varphi)$ varies by < 50% within the basal-plane [32], compared with > 300% in LSCO30. Hence, even if the small-angle scattering were dominant in Tl2201, it would have a much smaller effect on $R_H(0)$.

In summary, the Hall coefficient in overdoped LSCO is found to be extremely sensitive to details in the band structure and that in the absence of a change in carrier number or a FS modulation, interpretation of $R_H(T)$ requires the inclusion of strong in-plane anisotropy in the elastic scattering rate, presumably caused by small-angle scattering off out-of-plane Sr substitutional disorder. Very recently, strong (factor of 3 or more) variation in $\Sigma_0''(\varphi)$ of the AV symmetry was reported in LSCO over the entire doping range [33]. Our analysis of $R_H(T, x)$ affirms that this same form is manifest in the transport lifetime too. This striking violation of the isotropic-ℓ approximation, which may apply not only to the cuprates, but also to other 2D correlated systems, makes interpretation of $R_H$ in terms of carrier number highly inappropriate and misleading. It would certainly be instructive to learn what effect this will have on future interpretation of $R_H(T, x)$ in the underdoped regime.

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