Hall coefficient signals orbital differentiation in the Hund’s metal Sr$_2$RuO$_4$

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The Hall coefficient $R_H$ of Sr$_2$RuO$_4$ exhibits a non-monotonic temperature dependence with two sign reversals. We show that this puzzling behavior is the signature of two crossovers, which are key to the physics of this material. The increase of $R_H$ and the first sign change upon cooling are associated with a crossover into a regime of coherent quasiparticles with strong orbital differentiation of the inelastic scattering rates. The eventual decrease and the second sign change at lower temperature are driven by the crossover from inelastic to impurity-dominated scattering. This qualitative picture is supported by quantitative calculations of $R_H(T)$ using the Boltzmann transport theory in combination with dynamical mean-field theory, taking into account the effect of spin–orbit coupling. Our insights shed new light on the temperature dependence of the Hall coefficient in materials with strong orbital differentiation, as observed in Hund’s metals.

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INTRODUCTION
Measuring the Hall coefficient $R_H$ is a standard way of characterizing charge carriers in quantum materials. For free carriers of a single type, the Hall coefficient $R_H$ is simply given by the inverse of the density of carriers $n$ and their charge $e$. In principle, $R_H$ is negative for an electron-like Fermi surface (FS) and positive for a hole-like FS, respectively. Sign changes of $R_H$ can occur, for example, if the FS evolves from an electron-like to a hole-like one with temperature. However, in complex materials with a FS composed of multiple sheets, interpreting $R_H$ can be more complicated and also provides richer information when both electron-like and hole-like carriers are present simultaneously. For instance, in the case of one hole-like and one electron-like FS sheet, the corresponding Hall coefficient is given by an average of $R_{H,e} < 0$ and $R_{H,h} > 0$:

$$R_H = \frac{\sigma_e^2 R_{H,e} + \sigma_h^2 R_{H,h}}{\sigma_e + \sigma_h},$$

weighted by the squares of the individual hole and electron conductivities, $\sigma_e$ and $\sigma_h$, respectively. Hence, the ratio of scattering rates between the two types of carriers enters in a key manner to determine both the overall sign and magnitude of the Hall coefficient.

The 4d transition metal oxide Sr$_2$RuO$_4$ is such a complex material: with low-energy bands built out of three Ru-3d$_x$ orbitals ($d_{xy}$, $d_{xz}$, $d_{yz}$) hybridized with O–2p states, it has a FS comprising two electron-like sheets, β and γ, and one hole pocket, α. Indeed, experiments$^{5-7}$ have observed a particularly intriguing temperature dependence of $R_H$ in Sr$_2$RuO$_4$, as depicted in Fig. 1. $R_H$ increases from a negative value of about $-1 \times 10^{-10}$ m$^2$ C$^{-1}$ at low temperatures (values between $-1.37 \times 10^{-10}$ and $-0.7 \times 10^{-10}$ m$^2$ C$^{-1}$ for $T \to 0$ have been reported$^{8,9}$) exhibit a sign change at $T_1 = 30$ K (in the cleanest samples), reaches a positive maximum at about 80 K, changes sign a second time around $T_2 = 120$ K, and eventually saturates to a slightly negative value for $T > 200$ K.

Shirakawa et al.$^7$ suggested early on that the rich temperature dependence of $R_H$ in Sr$_2$RuO$_4$ points to the multi-carrier nature of this material. This conclusion, reached by considering a Drude model with two types of carriers, was later refined in several works$^{9-11}$ using Boltzmann transport theory calculations for tight-binding models assuming scattering rates $1/\tau_{\nu} = A_\nu + B_\nu T$ for the different FS sheets $\nu = \{\alpha, \beta, \gamma\}$, with adjustable parameters $A_\nu$ and $B_\nu$. The overall take-home message of these phenomenological models is that $R_H$ is highly sensitive to the precise details of the FS sheets and also to the temperature and sheet dependence of the scattering rates.

Another remarkable experimental finding provides insight in interpreting the temperature dependence of $R_H$ by$^7$ adding small amounts of Al impurities: it has a drastic impact on the intermediate temperature regime such that $R_H$ no longer turns positive and instead increases monotonically from the low-$T$ to the high-$T$ limit, as indicated by dotted lines in Fig. 1. Arguably, the similarity of the low-$T$ values of $R_H$ for different impurity concentrations provides evidence that the elastic-scattering regime has been reached where $R_H$ is mainly determined by FS properties (see also ref.$^7$). In contrast, the temperature dependence itself must be due to inelastic scattering, possibly associated with electronic correlations.$^7$

In this work, we address this rich temperature dependence of $R_H$ in Sr$_2$RuO$_4$ and provide a clear interpretation of its physical meaning. We show that the two sign changes of $R_H(T)$ in clean samples are the signatures of two important crossovers in the physics of this material. The increase of $R_H$ upon cooling from high temperature signals the gradual formation of coherent

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quasi-particles, which is associated with a strong temperature dependence of the ratio of inelastic scattering rates between the $xy$ and $xz/yz$ orbitals. At low temperatures the decrease of $R_{\eta}$ is due to the crossover from inelastic to impurity-dominated scattering. These qualitative insights have relevance to a wide class of materials with orbital differentiation.

Our qualitative picture is supported by a quantitative calculation of $R_{\eta}(T)$ using Boltzmann transport theory in combination with dynamical mean-field theory (DMFT), taking into account the electronic structure of the material. The spin–orbit coupling (SOC) is found to play a key role, because it has a strong influence on the shape of the FS and also controls the manner in which the scattering rates associated with the different orbitals combine into $k$-dependent quasi-particle scattering rates at a given point on the FS.

**RESULTS**

Dependence on scattering rate ratios

The orbital dependence of scattering rates is crucial for the understanding of the Hall effect. Therefore, we introduce a localized basis set of $t_{2g}$-like orbitals $|\chi_m\rangle$ with basis functions labeled as $m=|xy, xz, yz\rangle$ using maximally localized Wannier orbitals constructed from the Kohn–Sham eigenbasis of a non-SOC density functional theory (DFT) calculation. We treat SOC by adding an atomic SOC term for the $t_{2g}$ subspace with an effective strength of $\lambda=200$ meV, which takes already into account the correlation enhancement of the SOC by a factor of about two into account. We assign scattering rates $\eta_{xy}$, $\eta_{xz}$, and $\eta_{yz}$ (due to crystal symmetries $\eta_{xy}=\eta_{yz}$) to each orbital, irrespective of the microscopic details of the underlying scattering mechanisms, which will be addressed at a later stage. Then, these scattering rates are converted into $k$-dependent scattering rates for each band $\nu$:

$$\eta_{\nu}(k) = \sum_{m} |\langle \chi_m(k)|\psi_{\nu}(k)\rangle|^2 \eta_{\nu m}. \tag{2}$$

The overlap elements $|\langle \chi_m(k)|\psi_{\nu}(k)\rangle|^2$ correspond to the orbital character of the eigenstates $|\psi_{\nu}(k)\rangle$ of the Hamiltonian at a given momentum $k$. The orbital character for points on the FS is shown in the inset of Fig. 2. With the Hamiltonian and the scattering rates $\eta_{\nu}(k)$, we calculate $R_{\eta}$ within Boltzmann transport theory using the BoltzTraP2 package. Further details on Eq. (2), the Hamiltonian construction and the transport calculations, are provided in the Methods section.

In the Boltzmann transport theory, $R_{\eta}$ only depends on the scattering rates through their ratio $\xi = \eta_{xy}/\eta_{xz}$ and not through their absolute magnitude; a point we verified in our calculations. This also implies that within the constant isotropic scattering rate approximation, that is, $\xi=1$, the full temperature dependence of $R_{\eta}$ cannot be explained. The calculated $R_{\eta}$ as a function of the scattering rate ratio $\xi$ is displayed in Fig. 2. Without SOC $R_{\eta}$ remains negative for all values of $\xi$ and approaches zero as $\xi \rightarrow 1$. In this limit the $y$ sheet drops out and the contributions of the hole-like $a$ sheet and electron-like $\beta$ sheet compensate each other. This means that it is not possible to explain the positive value of $R_{\eta}$ observed experimentally in clean samples for $T_1 < T < T_2$ (Fig. 1) without taking SOC into account. With SOC we observe a very different behavior of $R_{\eta}(\xi)$: it turns from negative to positive at $\xi \approx 2.6$. This is a result of two effects (see Fig. 2, inset): First, SOC changes the shape and size of the FS sheets, and second, it induces a mixing between different orbital characters, which varies for each point on the FS. Thus, the manner in which the scattering rates associated with the different orbitals combine into $k$-dependent quasi-particle scattering rates (Eq. (2) is controlled by the SOC. From the calculated dependence of $R_{\eta}(\xi)$ in the presence of SOC, we deduce that agreement with experiments would require $\xi$ to be smaller than 2.6 at high temperatures, increase above this value at $\sim T$, and then decrease again to reach a value close to unity at low temperatures.

Inelastic electron–electron scattering

We turn now to microscopic calculations by first considering inelastic electron–electron scattering ratios calculated with DMFT (see Methods). These calculations consider the $t_{2g}$ subspace of states with Hubbard–Kanamori interactions of $U=2.3$ eV and $J=0.4$ eV. The calculated $\xi(T)$ from inelastic scattering only is displayed in Fig. 3a. In agreement with previous studies, we find that the $xy$ orbital is less coherent than $xz/yz$ at all temperatures and $\eta_{xy} < \eta_{xz/yz}$ in Sr$_2$RuO$_4$. In Sr$_2$RuO$_4$ the crossover from the low-$T$ coherent Fermi liquid regime with $\xi \sim T$ to an incoherent regime with a quasilinear temperature dependence of the scattering rate is well documented and also manifested in deviations of the resistivity from a low-temperature quadratic behavior to a linear one. Importantly, this coherence-to-incoherence crossover as well as the corresponding coherence scales are strongly orbital dependent. When approaching the Fermi liquid regime ($T_\text{FL} \approx 25$ K) the scattering rate ratio reaches a value as large as $\xi \approx 3$ (Fig. 3a), but decreases rapidly upon heating with $\xi \approx 1.8$ at 300 K. We do not find a substantial
Fig. 3  Influence of inelastic electron–electron scattering on the temperature dependence of $R_H$. a Inelastic scattering rate ratios extracted from dynamical mean-field theory (DMFT) self-energies extrapolated to zero frequency (see Methods). The error bars represent the standard deviation of nine consecutive DMFT iterations. b $R_H(T)$ considering the DMFT inelastic electron–electron scattering rate ratios. c Scattering rates $\eta_i(\theta)$ on the three Fermi surface sheets $v = (\alpha, \beta, \gamma)$ for $k_s = 0$ along the angle $\theta$ from $0^\circ$ (I–M) to $45^\circ$ (I–X) under consideration of the orbital character shown in the right inset of Fig. 2. The scattering rates at 29 K (blue) are multiplied by a factor of 44, chosen such that $\eta_\gamma(45^\circ)$ coincides with the result at 310 K (red). d Color map of $R_H$ assuming constant sheet-dependent scattering rate ratios. The solid black line indicates $R_H = 0$ and the dashed black line marks $\eta_\alpha = \eta_\beta$.

Connecting these results to the discussion of Fig. 2 above, the temperature dependence of $\xi$ directly translates into that of $R_H$ as shown in Fig. 3b. Like in experiments, $R_H$ is negative at high temperatures, but when the temperature is lowered it increases and crosses zero at 110 K. This demonstrates that electronic correlations are indeed able to turn $R_H$ positive and suggests the following physical picture: the electronic transport in Sr$_2$RuO$_4$ crosses from a regime governed by incoherent electrons at high temperatures, connected to a weaker orbital differentiation of scattering rates and a negative $R_H$ over to a coherent Fermi liquid regime, with a stronger orbital differentiation and positive $R_H$. The resulting sign change at 110 K can be seen as a direct consequence of this coherence-to-incoherence crossover. We emphasize that this sign change is only observed when SOC is taken into account. Without SOC $R_H$ is purely negative and shows only a weak temperature dependence (Fig. 3b, dashed line).

When moving along the FS from I–M ($\theta = 0^\circ$) to I–X ($\theta = 45^\circ$), the mixing of the orbital character induced by SOC (Eq. (2)) leads to angular-dependent scattering rates $\eta_i(\theta)$ (Fig. 3c). At $\theta = 0^\circ$ the ratio of scattering rates between the $\gamma$ and $\beta$ sheets is large, because these bands still have mainly $xy$ and $xz/yz$ character, respectively (Fig. 2, inset). As expected from Fig. 3a, this sheet dependence decreases with increasing temperature. On the other hand, at $\theta = 45^\circ$ the ratio is small, due to a very similar orbital composition of the $\gamma$ and $\beta$ sheets. The $\alpha$ pocket (being almost entirely $xz/yz$) has the lowest scattering rate and turns $R_H$ positive when $\xi$ becomes large enough at low temperatures. To shed more light on the interplay of the individual FS sheets, we can phenomenologically assign constant scattering rates to each FS sheet, as shown in Fig. 3d. We see that for $R_H$ to be positive a necessary condition is $\eta_\beta > \eta_\alpha$. This again highlights the importance of SOC, because without SOC the $\alpha$ and $\beta$ sheets have entirely $xz/yz$ orbital character, and thus $\eta_\alpha = \eta_\beta$. Should one make this assumption also in the presence of SOC, it would not result in $R_H > 0$ for any ratio $\eta_\gamma/\eta_\beta$ (Fig. 3d, dashed line).

Impurity-dominated scattering

Considering inelastic scattering only would yield a positive $R_H$ at even lower temperatures deep in the Fermi liquid regime. However, at such low temperatures elastic scattering is expected to dominate over inelastic scattering. The extracted DMFT scattering rates at 29 K with 5.5 meV for the $xy$ and 1.9 meV for the $xz/yz$ orbitals are of the order of the impurity scattering for “clean” samples with residual resistivities of $\sim 0.5 \mu\Omega\text{cm}$. Therefore, we add a constant elastic scattering $\eta_{el}$ to the orbital-dependent inelastic scattering $\eta_{inel}$. This elastic term is assumed to be isotropic: $\eta_{el} = \eta_{el}^{xy} = \eta_{el}^{xz/yz}$. The resulting temperature dependence of $R_H$ for values of $\eta_{el}$ ranging from 0.1 to 10 meV is shown in Fig. 4. The dashed lines are calculated with the Fermi liquid form $\eta_{inel}^{fl} = A_{\mu} T^2$ and parameters $A_{\mu}$ determined from the calculated inelastic scattering rates at 29 K.

For small enough $\eta_{el}$ we observe a second zero crossing of $R_H(T)$ and a regime with $R_H < 0$ at low temperatures, which is consistent with $R_H(T)$ depicted in Fig. 1. For $T \to 0$ the fully elastic-scattering regime is reached, and thus $R_H$ is not influenced by the magnitude of the (isotropic) scattering rate, but rather by the shape of the FS only. This regime corresponds to $\xi = 1$ in Fig. 2, for which we obtain $R_H = -0.94 \times 10^{-10} m^3 C^{-1}$, in good quantitative agreement with experiments. With increasing temperature the influence of elastic scattering fades away and the precise interplay with inelastic scattering shapes the overall temperature dependence of $R_H$. Hence, we see that also the low-temperature zero crossing has a simple physical interpretation: it signals the crossover between the regime dominated by elastic scattering at low temperatures and the regime dominated by inelastic
scattering at higher temperatures. Matching the two terms in the scattering rate, a simple estimate of the corresponding crossover scale is $T_1 \sim \sqrt{\eta^{\text{el.}}}/A_{2g} \sim \sqrt{\eta^{\text{el.}}} T_{\text{FL}}$. This scale obviously depends on the elastic-scattering rate, and coincides approximately with the Fermi liquid coherence scale $T_{\text{FL}}$ only for the cleanest samples reported in which $\eta^{\text{el.}} \sim T_{\text{FL}}$. For even cleaner samples we predict $T_1 < T_{\text{FL}}$.

On the contrary, for larger $\eta^{\text{el.}}$ we find that $R_H(T)$ ceases to exhibit any zero crossing and is negative in the whole temperature range. Only in very clean samples can the inelastic scattering rate sufficiently exceed the elastic one for the sign changes of $R_H$ to occur. This is further substantiated by experimental Hall measurements for samples where the residual resistivity was altered by introducing different amounts of Al impurities, cf. the dependence of $R_H$ on $\eta^{\text{el.}}$ in Fig. 4 and the inset with experimental data from ref. 7.

In the high-$T$ limit, we obtain a value of $R_H$ which is more negative and temperature dependent than the one reported in experiments. 5,7 Within the Boltzmann transport theory this would imply that a larger ratio $n_{\uparrow}/n_{\downarrow}$ is needed. Likewise, resistivities are significantly underestimated in DMFT transport calculations for $T > 300$ K in this material. 24 A possible explanation is that other sources of inelastic scattering, for example, electron–phonon scattering, could play an important role in the high-$T$ regime. We emphasize, however, that all experimental evidence points towards negligible magnetic contribution (due to processes like skew scattering) and a standard orbital-dominated Hall effect in Sr$_2$RuO$_4$.

**METHODS**

Hamiltonian and SOC

We use a maximally localized Wannier function construction to obtain an effective low-energy Hamiltonian for the three $e_g$-like orbitals centered on the Ru atoms. This construction is based on a non-SOC DFT calculation, using the software packages WIEN2k [41] and wien2wannier [43] with GGA-PBE [42] and wannier90 [44]. We incorporate the SOC as an additional local term, and add elastic scattering.

Inelastic scattering at higher temperatures. Matching the two terms in the scattering rate, a simple estimate of the corresponding crossover scale is $T_1 \sim \sqrt{\eta^{\text{el.}}}/A_{2g} \sim \sqrt{\eta^{\text{el.}}} T_{\text{FL}}$. This scale obviously depends on the elastic-scattering rate, and coincides approximately with the Fermi liquid coherence scale $T_{\text{FL}}$ only for the cleanest samples reported in which $\eta^{\text{el.}} \sim T_{\text{FL}}$. For even cleaner samples we predict $T_1 < T_{\text{FL}}$.

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**DISCUSSION**

In summary, our quantitative calculations and qualitative interpretations explain the highly unusual temperature dependence of the Hall coefficient of Sr$_2$RuO$_4$. The high-$T$ sign change of $R_H(T)$ in clean samples is the direct consequence of the crossover from a high-$T$ incoherent regime to a coherent regime with orbital differentiation. The orbital composition of each quasiparticle state on the FS, as well as the distinct scattering rates of the different orbitals, is crucial to this phenomenon and are properly captured by DMFT. This is in line with recent insights from angle-resolved photoemission spectroscopy. 16 In turn, the low-$T$ sign change is due to the crossover from inelastic to impurity-dominated scattering, which is further substantiated by comparing our results to experimental data on samples with a higher impurity concentration. Because it directly affects the shape of the FS sheets and strongly mixes their orbital character, SOC is found to be essential in explaining $R_H(T)$.

Orbital differentiation is actually a general feature common to Hund’s metals, 23,29–32 a broad class of materials in which the electronic correlations are governed by the Hund’s coupling, comprising for example transition metal oxides of the 4$d$ series as well as iron-based superconductors. 33–36 We note that a non-monotonic temperature dependence of the Hall coefficient has also been reported for Sr$_2$RuO$_4$. 76 Beyond ruthenates, LiFeAs and FeSe are two compounds without FS reconstruction due to long-range magnetic order, which display striking similarities to Sr$_2$RuO$_4$ in many regards. The FS of these superconductors is also composed of multiple electron- and hole-like sheets with distinct orbital composition and strong orbital differentiation. 31,32 Indeed, the Hall coefficient of LiFeAs has a strong temperature dependence 77 and that of FeSe displays two sign changes in the tetragonal phase. 39,40 These examples show that strongly correlated materials with multiple FS sheets of different or mixed orbital character and a orbital-differentiated coherence-to-incoherence crossover are expected to show a pronounced temperature dependence of the Hall coefficient. Sign changes then emerge in materials with balanced electron and hole-like contributions. These observations point to a wide relevance of our findings beyond the specific case of Sr$_2$RuO$_4$.
DATA AVAILABILITY

All data generated and analyzed during this study are available from the corresponding author upon reasonable request.

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AUTHOR CONTRIBUTIONS

M.Z. performed all calculations and the results were analyzed by M.Z. and A.G. All authors discussed and interpreted the results at different stages. The whole project was initiated by A.G. The manuscript was written by M.Z. with the help of all authors.

ADDITIONAL INFORMATION

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