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Orbital Dependence of the Fermi Liquid State in Sr$_2$RuO$_4$


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We have used angle-resolved photoemission spectroscopy to determine the bulk electronic structure of Sr$_2$RuO$_4$ above and below the Fermi liquid crossover near 25 K. Our measurements indicate that the properties of the system are highly orbital dependent. The quasi-2D $\gamma$ band displays Fermi liquid behavior while the remaining low energy bands show exotic properties consistent with quasi-1D behavior. In the Fermi liquid state below 25 K, the $\gamma$ band dominates the electronic properties, while at higher temperatures the quasi-1D $\beta$ and $\alpha$ bands become more important.

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The physics of low dimensional systems is determined by their electronic structure near the Fermi level. The low energy excitations in these states can give rise to exotic phenomena such as Mott insulators [1], charge and spin density waves [2], and high temperature superconductivity [3]. Sr$_2$RuO$_4$, known for being the only perovskite superconductor without Cu-O planes [4], is a particularly interesting example. Unlike the cuprates, which at optimal doping enter the superconducting phase from a non-Fermi liquid state, strontium ruthenate is known to show Fermi liquid properties well above the superconducting transition. The electronic structure in this material is actually quite complex, with three bands that are either quasi-one- or two-dimensional depending on their orbital symmetry [5].

The normal state transport in Sr$_2$RuO$_4$ is defined by two distinct phases. Below 25 K, the system acts like a simple anisotropic metal, although with strong electron correlations. The $T^2$ dependent resistivity [6] and linear specific heat [7] are well described by Fermi liquid theory. It is very unusual to witness these Fermi liquid properties in transport, as in simple metals these excitations are overwhelmed by electron-phonon interactions. As the temperature is raised, the system undergoes a broad crossover, and the system shows distinct non-Fermi liquid behavior. A temperature dependent anisotropy between the $c$ axis and in-plane transport properties is developed, resulting in a fully 2D material with a peak in the $c$-axis resistivity near 130 K and an in-plane resistivity with a linear $T$ dependence with no signs of saturation at the highest temperatures [8]. This transformation from a highly anisotropic Fermi liquid to a bad metal much like the normal state seen in the high-$T_C$ cuprates indicates that the scattering mechanisms are very different between the high and low temperature phases.

While dimensional crossovers of this sort are well known in low dimensional materials [9], Sr$_2$RuO$_4$ is a somewhat unique case owing to the nature of its electronic structure. The carriers in the system arise from three Ru $t_{2g}$ states, forming the Fermi surface shown in Fig. 1(a). The $d_{xz}$ and $d_{yz}$ orbitals make up the highly 1D bands $\beta$ and $\alpha$, while the 2D $\gamma$ band arises from the $d_{xy}$ orbital [5,10]. Because the interactions between the 1D and 2D bands are very weak, there are several aspects of the system that arise from either one or the other subset, such as the nature of the superconducting ground state [11], ferromagnetic excitations from $\gamma$ [12], and antiferromagnetic excitations due to nesting between $\alpha$ and $\beta$ [10,13].

![Fig. 1](image_url)

**FIG. 1.** (a) Schematic Fermi surface of Sr$_2$RuO$_4$. (b) Photoemission spectra taken along the $\Gamma$-$M$ direction from the freshly cleaved sample. Both surface ($S_\parallel$ and $S_\perp$) and bulk $\beta$ and $\gamma$ contributions can be seen. (c) MDC’s taken at the Fermi level (after the suppression of the surface state) at the beginning and end of the experiment. (d) Spectra taken after aging process with only bulk contributions remaining.
Angle-resolved photoemission spectroscopy is the natural probe for measuring characteristics of the electronic structure in order to identify the interactions that give rise to the exotic normal state properties of Sr$_2$RuO$_4$. The technique directly measures individual properties of the occupied band structure, including the dispersion, Fermi level crossing, and lifetime of each state. Performing these measurements at temperatures near the beginning of this crossover, between 10 and 60 K, we find that the temperature dependence of the transport scattering rate is strongly affected by the dimensionality and orbital symmetry of the band structure. The Fermi liquid state seen below 25 K can be correlated to quadratic energy and temperature dependencies in the lifetime of the 2D $\gamma$ band, while the anomalous transport behavior seen at high temperatures appears to arise from excitations in the 1D bands.

The photoemission experiments were performed in a UHV chamber with base pressure less than $1 \times 10^{-10}$ Torr at the undulator beam line U13UB of the National Synchrotron Light Source at Brookhaven National Laboratory. All photoemission spectra were taken with a photon energy of 15.2 eV using a Scienta SES200 analyzer. The total energy resolution was set to $\sim 25$ meV with an angular resolution of approximately $\pm 0.1$ degrees. The Sr$_2$RuO$_4$ single crystals used in this study were grown by the traveling floating zone method. The samples were oriented to an accuracy of $\sim 1^\circ$, or 0.03 Å$^{-1}$. During the study, the sample orientation deviated by less than 0.5$^\circ$ for spectra taken at various temperatures.

One major concern when attempting to correlate bulk properties of a material with photoemission measurements is the extremely short mean free path of photoexcited electrons. Because the measured electrons arise only from the first couple of layers, and the surface electronic structure may differ greatly from the bulk, one must be careful in applying the technique to bulk measurements. This surface sensitivity has been especially problematic for photoemission studies in Sr$_2$RuO$_4$, as a well-known surface reconstruction significantly alters the band structure in the first layer [14,15]. The influence of the surface can be seen in Fig. 1(b), with contributions from both surface and bulk features in the spectrum. The surface reconstruction causes the van Hove singularity of the surface $\gamma$ band to shift below the Fermi level and also shifts the Fermi level crossing of the $\beta$ band. The resultant spectrum is thus made up of four states (bulk and surface components) rather than the expected two making it almost impossible to quantitatively analyze the bulk electronic structure.

Fortunately, we are able to suppress the surface contributions by aging the sample in ultrahigh vacuum ($\sim 1 \times 10^{-10}$ Torr), resulting in bulk-only spectra as seen in Fig. 1(d). The spectra are then highly stable with respect to both aging time and temperature cycling, allowing for a quantitative temperature dependent analysis of the spectra. A constant energy cut of the spectra at the Fermi level taken at the beginning and end of the temperature dependent measurements of the bulk electronic structure is shown in Fig. 1(c). The spectral features remain completely unchanged over the time in which the experiment was performed. The only drawback to our aging process is that the spectra are considerably broadened with respect to freshly cleaved samples, most likely due to increased disorder in the system.

Confirming the bulk nature of the spectra, the measurements are in good agreement with respect to previous investigations of the system. The Fermi level crossings agree to within 0.05 Å$^{-1}$ with de Haas–van Alphen studies [16], theoretical calculations [5,14], and previous bulk photoemission investigations [15]. While it is difficult to determine the velocity of the bands exactly at the Fermi level owing to their width, the dispersion at higher binding energies agrees well with the local density approximation calculations [14].

Analysis of the photoemission spectra is performed by dividing the full 2D spectra [as in Figs. 1(b) and 1(c)] into constant energy cuts known as momentum distribution curves (MDC’s) [17]. The peaks as measured by MDC’s can be directly related to the inverse lifetime $\Gamma = \hbar/\tau$ via the relation of the peak width $\Delta k = \Gamma/v_0$ where $v_0$ is the bare velocity at the Fermi level and $\tau^{-1}$ is the scattering rate. Scans were taken along $\overline{\Gamma M}$ near the Fermi level crossings of $\beta$ and $\gamma$ so that measurements of each band could be performed simultaneously. Although not shown, the characteristics of $\alpha$ and $\beta$ are qualitatively similar.

Analysis of spectra taken over a range of binding energies and temperatures reveals that the Fermi level crossings and band velocities show no temperature dependence. Figure 2(a) shows a series of MDC’s at the Fermi level...
The Fermi level crossings of the $\gamma$ and $\beta$ bands are clearly visible as peaks in the spectra. The only obvious difference in the spectra is an increasing width in the line shape of the $\gamma$ band with increasing temperature. Examination of the line shape as a function of binding energy at 10 K [Fig. 2(b)] reveals that both peaks increase in width as the states disperse away from the Fermi level. Unfortunately, the peaks begin to overlap around 40 meV, making quantitative analysis of states at high binding energies impossible.

The inverse lifetime as a function of temperature and binding energy is shown in Fig. 3. The $\gamma$ and $\beta$ bands show drastically different characteristics. While the inverse lifetime of the $\beta$ band shows very little temperature dependence in this regime and a linear energy dependence, $\gamma$ has a far more complicated behavior. As can be seen in Figs. 3(a) and 4, the inverse lifetime of $\gamma$ appears to have a quadratic dependence on $\omega$ at low temperatures and $T$ at small energies, with the temperature dependence diminishing at higher binding energies. That two bands so near each other in the Brillouin zone act so differently is very surprising and confirms that the bands interact only weakly, with the nature of each state likely defined by very different interactions.

Examination of the seemingly complicated behavior seen in $\gamma$ reveals that the band is actually a well-defined two-dimensional Fermi liquid. The lifetime is proportional to $\omega^2 \ln(\omega)$ at the lowest temperatures and $(\pi k_B T)^2 \times \ln(k_B T)$ near the Fermi level. While the fit quality suffers only a little using the simple quadratic dependence expected for a 3D system, the large degree of anisotropy in Sr$_2$RuO$_4$ makes the two-dimensional form more appropriate. At finite temperature and binding energy, the lifetime dependence is more complicated, with the temperature (energy) dependence decreasing at higher binding energies (temperatures). This behavior is expected in a Fermi liquid state [18]. The combined temperature and energy dependence is well fit using $\Gamma = \Gamma_{\text{imp}} + \max[A_\omega \omega^2 \ln(\omega), A_T (\pi k_B T)^2 \ln(k_B T)]$ with $\Gamma_{\text{imp}}$ representing impurity scattering and the scaling factor $A_T \sim 2 A_\omega$.

On the other hand, $\beta$ shows no signs of Fermi liquid behavior. The lifetime is given by $\Gamma \approx \Gamma_{\text{imp}} + \omega$ (the slope is similar to that of $\alpha$), with almost no temperature dependence below 60 K (Fig. 4). The spectral weight of the peak does decrease slightly with temperature, but it is not clear how this impacts the properties of the system. Unfortunately, the $\beta$ band cannot simply be classified as a Luttinger liquid state, either. The band shows no signs of power law behavior in the density of states as it approaches the Fermi level, and there is no sign of asymmetry in the MDC’s as would be expected for spin-charge separation [Fig. 2(b)]. While $\beta$ shows some aspects of quasi-1D behavior, it is most likely not a purely one-dimensional state.

As the temperature is raised from 25 K, the scattering rate in the $\gamma$ band increases sharply, almost doubling by 70 K. Combined with a lack of significant broadening in $\beta$, this indicates the quasi-1D bands play a larger role in the transport properties of the system at higher temperatures, while $\gamma$ dominates at low temperatures. This is consistent

![Graphs](image-url)

**FIG. 3.** Inverse lifetime dependence of $\gamma$ and $\beta$ as a function of both temperature and binding energy. Data is plotted as symbols with error bars resulting from fits to the MDC’s. (a) The fits from 2D Fermi liquid theory are plotted as solid lines. (b) The solid line is a linear fit to the data at all temperatures.
The crossover seen in the transport properties is directly linked to these characteristics, giving rise to a scattering rate that is not only temperature dependent, but symmetry dependent as well. Although the exact nature of the excitations that cause these differences remains unclear, they are likely reflected in the magnetic properties of the system as well. Specifically, it appears likely that the non-Fermi liquid properties seen in the 1D bands are related to anti-ferromagnetic fluctuations, a similar situation as seen in the high-$T_c$ cuprates.

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**FIG. 4.** Temperature dependence of the lifetime of the $\gamma$ and $\beta$ bands at the Fermi level. Lifetime of $\gamma$. The solid line is a fit to the data from the $\gamma$ band according to 2D Fermi liquid theory. The dashed line is a linear fit to the data from the $\beta$ band.

with Hall coefficient measurements, in which a reduction in the mobility of the electron carriers from $\gamma$ could lead to $R_H$ becoming positive outside the Fermi liquid state [19,20]. Although the crossover is broad, with a large temperature regime where all bands strongly contribute to transport, it is clear that the Fermi liquid state is strongly linked to the properties of the 2D band while the non-Fermi liquid properties at high temperatures are derived by the nature of the 1D bands.

$\text{Sr}_2\text{RuO}_4$ has been shown to have a highly orbital dependent $p$-wave superconducting ground state [11,21]. Weak coupling between the 2D and 1D bands leads to different superconducting gaps, with the active $\gamma$ band defining the 1.5 K transition temperature. These findings are supported by specific heat measurements that show the existence of two gaps, the smaller of which can be related to the $\alpha$ and $\beta$ bands [22,23]. The photoemission measurements are in agreement with this picture, as the $\gamma$ band has much stronger interactions and plays a dominant role in determining the properties of the system at low temperature.

The symmetry dependent properties of the band structure are readily seen in the photoemission measurements.