Transport and the Order Parameter of Superconducting Sr$_2$RuO$_4$

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Recent experiments make it appear more likely that the order parameter of the unconventional superconductor Sr$_2$RuO$_4$ has a spin-triplet $f$-wave symmetry. We study ultrasonic absorption and thermal conductivity of superconducting Sr$_2$RuO$_4$ and fit to the recent data for various $f$-wave candidates. It is shown that only $f_{x^2-y^2}$-wave symmetry can account qualitatively for the transport data.

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The high-$T_c$-analog compound Sr$_2$RuO$_4$ poses a fundamental challenge to the study of unconventional superconductivity [1]. Clean samples become superconducting at about $T_c = 1.5K$ and the thermodynamics show that it is unconventional. The precise nature of its superconducting order parameter remains elusive, however. The simplest spin triplet case is the time-reversal-symmetry-breaking odd-parity $p$-wave state which has an order parameter $\Delta = \Delta(k_x + ik_y)$ [2]. Spin-triplet character is consistent with the Knight shift [3] and neutron scattering [4] measurements which indicate that the spin susceptibility shows no obvious suppression below $T_c$. Moreover, $\mu$SR experiment [5] confirms that the order parameter does indeed break time-reversal symmetry. The central feature of this $p$-wave order parameter is that it exhibits finite gap all over the Fermi surface (FS). However, more recent thermodynamic and transport measurements at low temperatures have found powers laws in the temperature dependences. This includes specific heat $C_V \propto T^2$ [6], Ru spin-lattice relaxation rate $1/T_1 \propto T^3$ [7], ultrasonic attenuation $\alpha \propto T^3$ [8], and thermal conductivity $\kappa \propto T^2$ [9,10]. These powers laws in $T$ are consistent with line nodes in the order parameter.

The combination of all experiments therefore favors the spin-triplet odd-parity $f$-wave symmetries which feature both time-reversal symmetry breaking and line nodes. Maki and Yang [11] have proposed an $f$-wave model with a superconducting order parameter $\mathbf{d}(T) = \Delta(T) \hat{z} k_z (k_x + ik_y)^2$ (the so-called “3D” model) for Sr$_2$RuO$_4$. This 3D gap has line nodes where the basal plane ($k_z = 0$) intersects the FS. It is similar to one of the leading candidates for the order parameter of UPt$_3$ (known as the $E_{g^*}$ model in that hexagonal system [12]). Graf and Balatsky [13] have proposed another candidate $f$-wave order parameter $\mathbf{d} = \Delta(T) \hat{z} (k_x + ik_y) k_y k_x$, which we will call the $f_{xy}$ model. This order parameter has line nodes perpendicular to the basal plane at where the planes $k_x = 0$ and $k_y = 0$ intersect the FS. This nodal structure is analogous to the $p$-wave model $\mathbf{d} = \Delta(T) \hat{z} \sin k_x + i \sin k_y$ proposed by Miyake and Nariykiyo [14]. It is suggested that $f_{xy}$-wave order parameter could arise from a pairing interaction mediated by antiferromagnetic spin fluctuations with peak intensities at the incommensurate wavevectors $\mathbf{q} = (\pm 2/3\pi, \pm 2/3\pi)$. The latter has been confirmed by inelastic neutron scattering [15]. Finally there is the $f_{x^2-y^2}$-wave order parameter $\mathbf{d} = \Delta(T) \hat{z} (k_x + ik_y) (k_x^2 - k_y^2)$ with line nodes where the planes $k_y = \pm k_x$ intersect the FS. This has been suggested [16] partly by analogy to high $T_c$ cuprates where a similar $x^2-y^2$ (but with spin-singlet) gap structure has been conclusively established. It is worth noting that the above three models all account reasonably well for the specific heat and superfluid density data [17,18].

The structure of all of these gaps in momentum space is rather complicated. Since all thermodynamic and transport quantities involve Fermi surface averages, it is not easy to see how they may be distinguished experimentally. In the study of heavy-fermion superconductors, it has been found that thermal conductivity and ultrasonic attenuation can be key tools in this situation. These quantities can be studied as a function of propagation direction and, in the case of the attenuation, also of polarization dependence. The key point is that this directional sensitivity can not only test for the presence of point or line nodes, but can also determine the positions of nodes and the orientations of nodal lines. These experiments [19,20] offer the best chance to distinguish between order parameters that have different nodal structures but share similar thermodynamic properties.

In this paper, we calculate the thermal conductivity and the transverse and longitudinal ultrasonic attenuation of Sr$_2$RuO$_4$. We consider the three major candidates of $f$-wave symmetry mentioned above, namely the 3D, $f_{xy}$, and $f_{x^2-y^2}$ models. It will be shown that only the $f_{x^2-y^2}$ model can account for the data even qualitatively. The in-plane $k_x^2-k_y^2$ symmetry offers an intriguing similarity to the high-$T_c$ order parameter. If this gap structure is indeed manifested in Sr$_2$RuO$_4$ it would suggest the presence of anti-ferromagnetic (AF) fluctuations in the ruthenate superconductors, perhaps peaked at or near $\mathbf{q} = (\pi, \pi)$ (such as one finds in the cuprates). The transport data thus suggests that AF fluctuation may also exist in ruthenates.

Ultrasonic attenuation experiments in Sr$_2$RuO$_4$ have been done in the hydrodynamic regime where the sound frequency $\omega$ satisfies $\omega << 1/\tau$, where $\tau$ is the electronic relaxation time [10]. In this case the Boltzmann equa-
solution is appropriate, and the attenuation $\alpha_{ij}$ for sound propagation along the direction $\hat{q} \parallel \hat{i}$ with polarization $\tilde{\varepsilon} \parallel \hat{j}$ is [21]:

$$\alpha_{ij}(T) \propto \int_0^\infty d\omega \left[ -\frac{\partial F(\omega)}{\partial \omega} \right] \tau_\eta(\omega, T) \times \left\langle \text{Re} \left( \frac{\sqrt{\omega^2 - |\mathbf{k}|^2}}{\omega} [(i \cdot \hat{k})(j \cdot \hat{k}) - \frac{1}{d}|\delta_{ij}|^2] \right) \right\rangle. \quad (1)$$

Here $d$ denotes the dimensionality, $F$ is the Fermi function, and the angle brackets indicate an FS average. Note the second term inside the square bracket vanishes for the transverse case. Similarly the thermal conductivity in the $i$th direction when a temperature gradient is imposed along the $i$th direction is computed using:

$$\kappa_i(T) \propto \frac{1}{T} \int_0^\infty d\omega \omega^2 \left[ -\frac{\partial F(\omega)}{\partial \omega} \right] \tau_s(\omega, T) \times \left\langle \text{Re} \left( \frac{\sqrt{\omega^2 - |\mathbf{k}|^2}}{\omega} (i \cdot \hat{k})^2 \right) \right\rangle. \quad (2)$$



The FS of Sr$_2$RuO$_4$ has been determined by de Haas-van Alphen experiments. It has three sheets denoted by $\alpha$, $\beta$, and $\gamma$ [23]. These are in good agreement with LDA calculations [23]. The bands are two-dimensional, a feature similar to cuprates. Among these three bands, the $\gamma$ band has the largest FS and has the highest density of states (DOS) at the Fermi energy. For simplicity, we use a single cylindrical FS for $f_{xy}$ and $f_{x^2-y^2}$ models and a three-dimensional spherical FS for the 3D model. We shall comment on the effects of FS anisotropy below. We will assume that the momentum dependence of the gap is independent of temperature, which leaves only the overall magnitude $\Delta(T)$. The temperature dependence of the gap in Sr$_2$RuO$_4$ has not been directly measured. However, one may deduce the power law at low temperatures from the pattern of nodes and near $T_c$ the power is given by mean field theory. For line nodes, a reasonable interpolation for the temperature dependence is $\Delta(T) = \Delta(0)[1 - (T/T_c)^{3/2}]^{1/2}$. This form has only one parameter $\Delta(0)$, reducing the arbitrariness in the fitting procedure.

Inspection of Eqs. (1) and (2) shows that the only remaining unknown is the relaxation time $\tau_s(T)$. Our procedure will be to use the thermal conductivity to determine the relaxation time and the magnitude of the ground state gap $\Delta(0)$, then use these to constrain the fits of the attenuation.

In Fig. 1 we show the best fits against the thermal conductivity $\kappa_\eta$ along the [100] direction in the normal and superconducting states. The normal state is achieved experimentally by applying a sufficiently strong external magnetic field. The data are those of Tanatar et al. [1]. In the normal state at $0.5T_c \lesssim T \lesssim T_c$, the scattering rate can be well described by an empirical form: $1/\tau_n = \Gamma_0(1 + aT^2/T_c^2)$ with $\Gamma_0 \simeq 0.01\pi T_c$ and $a = 0.15$. That is, the inelastic scattering rate is observed to be roughly 15% of the elastic part at $T_c$. For the effective scattering rate in the superconducting state, we take the same temperature dependence as in the normal state. This is clearly appropriate for $T \lesssim T_c$. At lower temperatures $T \ll T_c$, due to the opening of the gap, the inelastic rate could decrease faster than $T^2$. However, since the elastic scattering rate dominates over the inelastic part, the exact temperature dependence of inelastic rate is not so important. (This is one big difference between this system and the heavy fermion and high-$T_c$ materials.) Fitting to the superconducting thermal conductivity data then fixes the other parameter $\Delta(0)$. It turns out that all three theoretical candidates can fit the data for $\kappa_\eta$ in the superconducting state. There is no noticeable difference in goodness-of-fit for the different models. The parameters determined by the fits are $\Delta(0) = 1.65T_c$ for $f_{x^2-y^2}$ model, $\Delta(0) = 3.3T_c$ for $f_{xy}$ model, and $\Delta(0) = 4.05T_c$ for 3D model. The difference in size between these various values is not significant, since each gap form has a different relation between $\Delta(0)$ and the root-mean-square FS average gap. It is the latter quantity that is more important in determining the overall scattering strength.

The parameters determined by the fit in Fig. 1 are now used to calculate the transverse and longitudinal ultrasonic attenuation without any adjustable parameters (Fig. 2) for all three models.
This sets a crucial constraint on theoretical models. The 3D gap has an effective FS located near the nodes, with a polarization-dependent weighting factor. The averages therefore lead to \( \langle \hat{k}_x^2 \hat{k}_y^2 \rangle \) finite, while \( \langle (\hat{k}_x^2 - 1/d)^2 \rangle \equiv 0 \) (\( d = 2 \)) again, favoring transverse attenuation. These averages show that the \( f_{x^2-y^2} \) will naturally have more transverse attenuation than its competitors. Although we have plotted only one set of curves for each of the states, this is a general feature. The fact that the attenuation data favor \( f_{x^2-y^2} \) over other candidates was already noted by Lupien et al. [10] without calculation.

Since the data in Figs. 1 and 2 are taken on different samples (\( T_c = 1.44 \text{K} \) and 1.37 K, respectively), one does not expect a quantitatively good fit in Fig. 2 using the same parameters in Fig. 1. At first glance, our results of \( \alpha \) for \( f_{x^2-y^2} \) and \( f_{xy} \) waves are qualitatively similar to Graf and Balatsky’s [13] when a resonant scattering limit (\( \delta = 90^\circ \)) is taken under the self-consistent \( T \)-matrix approximation. Lupien et al. [14] pointed out that while the sound attenuation data favors \( f_{x^2-y^2} \) wave, the low \( T \) power law is much lower than the calculated result of Graf and Balatsky for the longitudinal case. In contrast, as shown in Fig. 2, our calculation based on a phenomenological input of scattering time gives satisfactory good fit for the longitudinal case including the low \( T \) power law. It also leads to better fit for the transverse case especially at \( T < T_c \), compared to Graf and Balatsky’s almost linear in \( T \) result. The still rather large discrepancy between the theoretical fits and the experimental data (especially for the T100 mode) could be due to the order parameter which is more involved than having the pure \( f_{x^2-y^2} \) symmetry. This remains to be studied in more details.

It is important to note one major difference between our phenomenological treatment and the self-consistent \( T \)-matrix approximation used by Graf and Balatsky. In the unitary limit, the usual \( T \)-matrix approximation for the impurity scattering will assume a strongly frequency dependent scattering rate \( 1/\tau_{\text{imp}} \sim 1/\omega \) in the superconducting state [15]. In contrast, we have adopted a constant elastic scattering rate (i.e., \( \Gamma_\parallel \)). Our phenomenological input relies truly on the good fit to the thermal conductivity data in the superconducting state (see Fig. 1).

In-plane thermal conductivity measured by Izawa et al. [12] with a rotating in-plane magnetic field has shown a four-fold pattern with a minimum when \( \mathbf{H} \parallel [110] \). This angle dependence is consistent with the \( f_{x^2-y^2} \) and 3D models but rules out the \( f_{xy} \) model [17]. In terms of variation of the amplitude, Izawa et al. claimed that the state \( \mathbf{d} = \Delta(T) \hat{z} (k_z + ik_y)(\cos c k_z + |b|) \), originally proposed by Hasegawa et al. [24], is more consistent with the data based on the approach in Refs. [10,11]. Here \( c \) is the spacing between two adjacent Ru layers and \( |b| \leq 1 \). This model has a circular-like line node parallel to the basal plane with any \( k_z \) satisfying \(-1 \leq k_z c \leq 1 \). This

![Figure 2](image-url)
gap is symmetrical for any given parallel $k$ plane and will lead to a sound attenuation very similar to that of the 3D model above. Thus it also does not produce the proper polarization dependence.

Finally we comment on the effect of Fermi surface anisotropy. While in Sr$_2$RuO$_4$ the FS has multiple sheets and there seems to be a coupling between the $\alpha$ and $\beta$ bands, the analysis of transport data given here will not be significantly modified providing that the $D_{4h}$ symmetry of the crystal is preserved. Moreover, our result for the 3D model stands if the spherical FS is replaced by an ellipsoidal one that has circular projection parallel to the basal plane. As long as transport data is concerned, it is likely that interband effects are unimportant.

In conclusion, the transport data of Sr$_2$RuO$_4$ presently give strong preference to the $f_{x^2-y^2}$-wave order parameters with perpendicular line nodes at $k_x = \pm k_y$. A sharper comparison of theory and experiment will be possible if the data for $\alpha$ and $\kappa$ is taken on the same sample. Furthermore, we suggest that the out-of-plane transverse sound attenuation measurement should be performed under the polarization $\hat{q} \parallel \hat{x}$ and $\hat{\varepsilon} \parallel \hat{z}$. This will shed more light on the information of the location of line nodes and the overall nodal structure.

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