Three Band Model for Superconductivity in Sr\textsubscript{2}RuO\textsubscript{4}

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Abstract

We analyse the pairing symmetry of the order parameter in superconducting Sr\textsubscript{2}RuO\textsubscript{4}. Basing on a realistic three dimensional 3 band energy spectrum we have introduced effective attractive electron-electron interactions and found a solution which has line nodes in the gap in $\alpha$ and $\beta$ bands but not in $\gamma$ band. This state breaks time reversal symmetry and leads to the proper temperature dependence of the specific heat, in-plane penetration depth and thermal conductivity.

1 Introduction

Sr\textsubscript{2}RuO\textsubscript{4} is an oxide with a lattice structure similar to the well known high temperature superconductor La\textsubscript{2-x}Ba\textsubscript{x}CuO\textsubscript{4} \cite{1, 2} with ruthenium replacing copper. When pure it becomes a superconductor at $T_c=1.5$K and is one of the best candidates for spin triplet superconductivity \cite{2, 3, 4}.

In spite of many convincing arguments for $p$–wave pairing the proper symmetry of three band superconducting order parameter is still unknown.

The muon spin rotation experiments \cite{5} indicate the existence time reversal symmetry breaking, consistent with the order parameter $\Delta(k) = i\vec{d}_y \vec{\sigma} \cdot \vec{d}(k)$, with $d(k) = (0,0,d^z(k))$ and $d^z(k) = \Delta(T)(k_x + ik_y)$. At the same time many thermodynamic properties show power low temperature dependences at low $T$, clearly pointing at the existence of nodes in the order parameter. The experiments on specific heat \cite{6}, penetration depth \cite{7} and thermal conductivity \cite{8} all show a quadratic dependence on temperature. This is surprising since a complete symmetry analysis of $p$–wave pairing in
tetragonal crystals shows no states which both break time reversal and possess line nodes [9, 10].

In the literature there exist a number of proposals for the relevant symmetry states [3, 4, 11, 12, 13, 14, 15, 16]. Most of them concentrate on two dimensional band models with p-wave symmetry states. Here we propose to start with the real three dimensional electron energy spectrum with all three bands (called α, β and γ) taken into account and allow for both in plane and out plane p-wave symmetries of the order parameter.

In the next section we present our Hamiltonian and the approach, which is the full solution of the Bogolubov - de Gennes equations at each point of the three dimensional Brillouin zone. In principle our theory does not contain free parameters. By fitting the calculated Fermi surface to the experimentally determined one we fixed the single particle parameters of the Hamiltonian. The remaining three interaction parameters have been fitted by requiring that all three bands have a single superconducting transition temperature (i.e. the monotonic low T behaviour of the specific heat) and a correct value of the transition temperature. Using the parameters we have solved the Bogolubov-de Gennes equations. The obtained gap functions have been used to calculate penetration depth and thermal conductivity.

2 The Symmetry of the Order Parameter

We start with the description of the electronic structure of Sr$_2$RuO$_4$ in the vicinity of the Fermi energy $\epsilon_F$ in the normal state. We consider three orbitals of ruthenium A, B, C of character $d_{xz}$, $d_{yz}$ and $d_{xy}$, respectively. These generate 3 Fermi surface sheets $\alpha$, $\beta$ and $\gamma$. The $\alpha$ and $\beta$ sheets arise from hybridised A and B orbitals which we model with hopping parameters ($t_1$, $t_2$, $t_{AB}$), which describe AA (BB) hopping in x(y) direction, AA (BB) hopping in y(x) direction and AB hopping, respectively. The $\gamma$ sheet arises from the C orbitals, which we model by hopping parameters $t$ and $t'$ for nearest and next nearest neighbour sites. We have fitted these parameters to the de Haas - van Alphen experimental cross-sections of the Fermi surface [17]. To allow for the three dimensional Fermi surface [18] we add the hopping parameter $t_\perp$ which we assume to take on the same value for each band.

Due to the symmetry of the orbitals and the body centered tetragonal symmetry of the crystal we assumed that the dominant pairing interactions
were in plane $U_\gamma$ for the $\gamma$ band, and inter-plane $U_{\alpha,\beta}$ for the $\alpha$ and $\beta$ bands. Each of these was tuned by fitting to the experimental superconducting critical temperature $T_C = 1.5$ K, so we have no free parameters.

Our strategy is to solve the Bogolubov-de Gennes equations to find the pairing potentials and energy spectrum. We allowed for the following general structure of the pairing potential

$$
\tilde{d}_{\nu,\nu'}^\pm(k) = \Delta_{\nu,\nu'} \sin k_x + \Delta_{\nu,\nu'} \sin k_y \\
+ \left[ \Delta_{\nu,\nu'} \sin (k_x/2) \cos (k_y/2) + \Delta_{\nu,\nu'} \sin (k_y/2) \cos (k_x/2) \right] \cos (k_z c/2) \\
+ \Delta_{\nu,\nu'} \sin (k_z c/2) \cos (k_y/2),
$$

in units where the lattice constant, $a = 1$, and where indices $\nu, \nu'$ take the values $\alpha, \beta, \gamma$. Each of these solutions therefore breaks the time-reversal symmetry. Moreover, due to the factor $\cos (k_z c/2)$ (Eq. 1) we have planes of zeros on the $\alpha$ and $\beta$ sheets for $k_z = \pm \pi/c$.

To illustrate the structure of the gap on the Fermi surface we have plotted in Fig. 1 the eigenvalues for the $\beta$ and $\gamma$ sheets. Figure (1a) illustrates clearly the zero eigenvalues in the $\beta$ band on the planes $k_z = \pm \pi/c$. The structure of the gap on the $\alpha$ sheet is very similar. Contrary to that the gap on the $\gamma$ band (Fig. 1b) is always finite but has strong modulation in the (x,y) plane.
The temperature dependence of the gap parameters is shown in Fig. 2a and the specific heat in Fig. 2b. The overall agreement with the experimental data is good. In particular the height of the step at $T_c$ and the linear dependence of $C/T$ on temperature agree with experiment [6].

For the above state we have also calculated the penetration depth $\lambda$ (Fig. 3a) and the thermal conductivity $\kappa$ (Fig. 3b). The penetration depth shows a close to linear dependence on temperature at low $T$ and agrees approximately with the experimental data [8]. Note that impurity scattering or other effects may change the low temperature power low. The thermal conductivity is quadratic as expected for a gap with line nodes.

3 Remarks and Conclusions

Using a realistic three band model of Sr$_2$RuO$_4$ we have found a $p$–wave pairing state which has nodes and breaks time reversal symmetry. The state has $^3E_u[e]$ (axial) pairing symmetry in the notation of [9]. The line node on the $\alpha$, $\beta$ sheets is a consequence of the specific form assumed for the pairing interaction.

The state we have found is of similar nature as the one proposed on different grounds in [13, 15]. Our model contains only attractive interactions unlike one proposed in [15]. The nice feature of our model is that we have no
adjustable parameters. The state we obtained leads to correct temperature dependence of not only specific heat but also the penetration depth and thermal conductivity.

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