Theory of spontaneous Fermi surface symmetry breaking for $Sr_3Ru_2O_7$

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Abstract

We show that many salient features observed around the metamagnetic transition in $Sr_3Ru_2O_7$ are described within a simple model, which considers only an instability of the Fermi surface symmetry breaking (Pomeranchuk instability), without invoking a putative metamagnetic quantum critical end point as usually assumed for this compound. In our model, the Pomeranchuk instability and unconventional, non-Fermi liquid type properties arise due to the tuning of the van Hove singularity of either a majority or minority band to the vicinity of the Fermi energy by a magnetic field. The obtained phase diagram, the metamagnetic transition, and the temperature dependence of the magnetic susceptibility and specific heat show striking similarities to the experimental data.

Key words: quantum critical points; Fermi surface; Pomeranchuk instability; metamagnetism
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$Sr_3Ru_2O_7$ is a bilayered material with metallic RuO_2 planes where the Ru ions form a square lattice. *Ab initio* calculations[1] showed that the electronic band structure is similar to that for the single layered ruthenate Sr_2RuO_4, a well-known spin-triplet superconductor. The ground state of $Sr_3Ru_2O_7$ is, however, paramagnetic. By applying a magnetic field h, $Sr_3Ru_2O_7$ shows a metamagnetic transition around $h = h_c$[2], where non-Fermi-liquid behavior was observed in various quantities such as the uniform magnetic susceptibility[3], specific heat[2,4,5], and resistivity[6]. These anomalous properties were often discussed in terms of an underlying metamagnetic quantum critical end point (QCEP)[7]. However, subsequent measurements for ultrapure crystals showed that the metamagnetic QCEP was not realized but instead some ordered phase was stabilized with a dome-shaped transition line[8]. While a second order transition was speculated to occur around the center of the dome, a first order transition was confirmed at the edges of the dome and was accompanied by a metamagnetic transition. Grigera *et al.*[8] discussed that spontaneous d-wave type Fermi surface symmetry breaking, namely the so-called d-wave Pomeranchuk instability, occurs inside the dome. This d-wave type Fermi surface deformation (dFSD) is a new type of spontaneous symmetry breaking in the sense that the Fermi surface breaks the point-group symmetry of the underlying lattice structure, which was first discussed in the t-J[9] and Hubbard[10] model in the context of high-temperature cuprate superconductors.

The possibility of a dFSD in $Sr_3Ru_2O_7$ is currently a hot topic. It is tempting to associate anomalous electronic properties in $Sr_3Ru_2O_7$ with the hypothetical metamagnetic QCEP, which is hidden by the dFSD instability. In this paper, however, we find that the van Hove singularity of the density of states can be of central importance to electronic properties in $Sr_3Ru_2O_7$. Within this scenario, the phase diagram of the dFSD instability, the metamagnetic transition, and the anomalous temperature dependence of the uniform magnetic susceptibility and specific heat coefficient, which show striking similarities to the experimental observations, are naturally obtained without invoking a putative metamagnetic QCEP.

We analyze a pure forward scattering model driving the dFSD in the presence of a magnetic field,

$$H = \sum_{\mathbf{k},\sigma} (\epsilon^0_{\mathbf{k}} - \mu)\, n^\sigma_{\mathbf{k}} + \frac{1}{2N} \sum_{\mathbf{k},\sigma,\mathbf{k}',\sigma'} f_{\mathbf{k}\mathbf{k}'}\, n^\sigma_{\mathbf{k}} n^{\sigma'}_{\mathbf{k}'} - h \sum_{\mathbf{k},\sigma} \sigma n^\sigma_{\mathbf{k}}\,, \quad (1)$$

where $n^\sigma_{\mathbf{k}} = c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$ is the number operator of electrons with momentum $\mathbf{k}$ and spin σ; μ is the chemical potential; N is the number of lattice sites; h is the magnetic field. For hopping amplitudes t and t' between nearest and next-nearest neighbors on a square lattice, respectively, the bare dispersion relation is given by $\epsilon^0_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y$. The forward scattering interaction driving the spontaneous dFSD has the form $f_{\mathbf{k}\mathbf{k}'} = -g\, d_{\mathbf{k}} d_{\mathbf{k}'}$ with

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a coupling constant $g \geq 0$ and a d-wave form factor $d_{\mathbf{k}} = \cos k_x - \cos k_y$. This ansatz mimics the structure of the effective interaction in the forward scattering channel as obtained for the t-J[9] and Hubbard model[10].

We decouple the interaction by introducing a spin-dependent mean field $\eta^\sigma = -\frac{g}{N}\sum_{\mathbf{k}} d_{\mathbf{k}} \langle n_{\mathbf{k}}^\sigma \rangle$ and obtain a renormalized band dispersion $\xi_{\mathbf{k}}^\sigma = \epsilon_{\mathbf{k}}^0 + \eta d_{\mathbf{k}} - \mu^\sigma$ with $\eta = \sum_\sigma \eta^\sigma$; the mean fields are determined by minimizing the free energy, which is an even function with respect to η, and the solution with $\eta \geq 0$ is considered. The magnetic field is absorbed completely in the effective chemical potential $\mu^\sigma = \mu + \sigma h$. Since the Hamiltonian (1) does not allow momentum transfer, the mean-field theory solves our model exactly in the thermodynamic limit.

Figure 1(a) shows the phase diagram in the plane of the applied magnetic field h and the temperature T; we take the parameters $t'/t = 0.35$, $\mu/t = 1$, and $g/t = 1$, and set $t = 1$. The dFSD transition occurs around the van Hove energy of the up-spin band ($h = 0.4$) with a second order transition for high T and a first order one for low T, which is very similar to the phase diagram reported by Grigera *et al.*[8] In Fig. 1(b) we show the h dependence of the order parameter η, together with η^σ, at low T. Both $\eta^\uparrow$ and $\eta^\downarrow$ show a jump at the first order transition point, but with a different magnitude. The FSs at low T are shown in Fig. 1(c) for $h = 0.35$. The gray lines are FSs for $g = 0$ and the outer (inner) FS corresponds to the up-spin (down-spin) band. The FS instability drives a deformation of both FSs and typically leads to an open outer FS. The first order dFSD instability is generically accompanied by a metamagnetic transition, since the grand canonical potential must be a concave function of h.

Around the van Hove filling, the uniform magnetic susceptibility χ has a strong T dependence and forms a pronounced peak at low temperature, which is very similar to the T dependence observed in the experiment[3]. The dFSD instability then cuts off such non-Fermi liquid like behavior of χ and produces a cusp at the second order transition temperature. The specific heat coefficient γ has a peak at low T with a $\log T$ divergence at the van Hove energy, which is also very similar to the behavior observed experimentally[2,4,5]. The dFSD instability produces a jump in the specific heat at the second order transition temperature. Further details of the T dependence of χ and γ are discussed in Ref. [11].

In summary, the most salient features observed in $Sr_3Ru_2O_7$ are well captured in terms of the dFSD instability near the van Hove filling. When either the majority or minority band is tuned to the van Hove filling by the magnetic field, the dFSD instability occurs in both bands, but with a different magnitude of the order parameter. The transition is of second order at high T and changes to first order at low T. The first order transition is accompanied by a metamagnetic transition. Both the magnetic susceptibility and the specific heat coefficient show strong T dependences near the van Hove filling. This non-Fermi liquid behavior originates from the van Hove singularity in the density of states of the bare dispersion and is cut off by the dFSD instability.

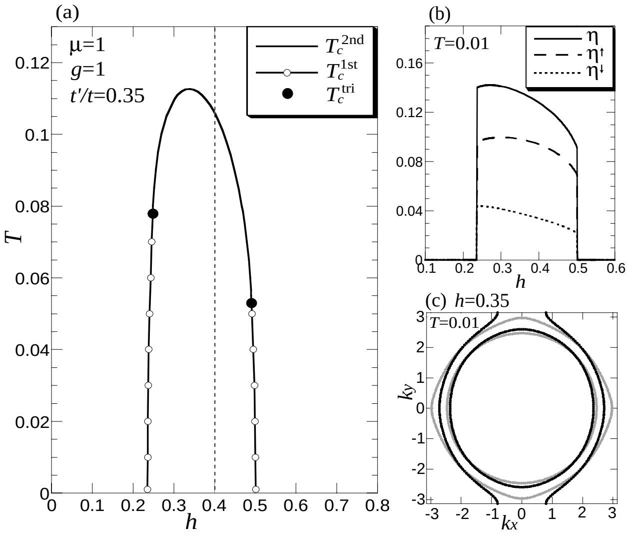

Fig. 1. The mean-field results for $\mu = 1$ and $g = 1$. (a) The dFSD phase diagram in the plane of magnetic field h and temperature T; the solid line and open circles denote second and first order phase transition, respectively; end points of the second order line are tricritical points. The dotted line ($h = 0.4$) represents the van Hove energy of the up-spin band. (b) The h dependence of the order parameter; note that $\eta = \eta^\uparrow + \eta^\downarrow$. (c) The FSs for $g = 1$ (solid line) and 0 (gray line) at $h = 0.35$; the deformation of the inner FS is hardly visible.

$Sr_3Ru_2O_7$ is often referred to as a system with a metamagnetic QCEP. In our model, the metamagnetism originates from the first order dFSD transition. Since the dFSD transition does not lead to a QCEP in our model, it remains to be studied whether a concept of a metamagnetic QCEP can be really a good basis to discuss anomalous properties in $Sr_3Ru_2O_7$. In this sense, it is important to clarify whether the anomalous T dependence of the resistivity observed around the metamagnetic transition[2] can be explained in terms of dFSD fluctuations and the van Hove singularity or whether we have to invoke quantum fluctuations originating from some QCEP.

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