Slave-boson mean-field study of the dimensional crossover in Sr$_2$RuO$_4$

M H Fischer and M Sigrist
Theoretische Physik, ETH Zürich, 8093 Zürich, Switzerland
E-mail: mfischer@itp.phys.ethz.ch

Abstract. The anomalous temperature dependence of the $c$-axis resistivity of Sr$_2$RuO$_4$ is analyzed under the viewpoint of a dimensional crossover which occurs from a lattice of perpendicular one-dimensional chains, belonging to different Ru-4d-orbitals, to a two-dimensional system induced by weak inter-orbital hybridization. This system is described by a two-orbital Hubbard model which is treated within a slave-boson mean-field approach to take correlation effects, such as the spin-charge separation, into account. We obtain the emergence of quasiparticle states at low temperature, a result which can be used to discuss the evolution of the spectral density and the $c$-axis transport within a tunneling approach. For the latter, a crossover between the low- and high-temperature regime is found in qualitative agreement with experimental observations.

1. Introduction
Correlation effects among electrons lead to strong modifications of the electronic spectrum especially in low dimensions. In one dimension, electrons can even separate into independent spin and charge degrees of freedom. As all solids are three-dimensional, low-dimensionality appears only through highly anisotropic electronic properties governed by crystal and electronic orbital structures. Often an effective dimensionality results from the difference of energy scales. This can give rise to changes of the dimension, a dimensional crossover, when system parameters are changed [cf. Fig. 1a)]. Consequences include highly complex phase diagrams known from many organic materials and qualitative changes of transport properties which can be connected with a modification of the nature of charge carriers. We argue here that Sr$_2$RuO$_4$, which is a quasi-two-dimensional strongly correlated Fermi liquid particularly well-studied for its unconventional superconducting phase[1], is an example with such behavior. The tetragonal layered perovskite crystal structure of Sr$_2$RuO$_4$ gives rise to a strong anisotropy of the electrical resistivity between in-plane and out-of-plane current direction: $\rho_c/\rho_{ab} \sim 10^3$ at $T = 2$K. The $c$-axis transport shows an anomalous temperature dependence. While it is Fermi liquid-like at low temperatures, a crossover from metallic to insulating temperature dependence occurs around $T^* \approx 130$K [2]. Because no structural or other ordering phenomena accompany this change, it has been attributed to strong electron correlations.

We propose here a mechanism based on a dimensional crossover within the basal plane which affects the interlayer transport through the change of the quasiparticle nature. The band structure is well described by a tight-binding model including the three 4$d$-$t_{2g}$-orbitals on the lattice of the Ru-ions, which have $\pi$-hybridization with the O-2$p$-orbitals[3, 4]. We
concentrate here on the two orbitals \( d_{yz} \) and \( d_{zx} \), most relevant for the \( c \)-axis transport which we assume to be due to inter-layer tunneling. For both orbitals, nearest-neighbor intra-orbital \( \pi \)-hybridization yields essentially one-dimensional (1D) bands. An inter-orbital coupling occurs through much weaker next-nearest-neighbor hybridization between \( d_{yz} \) and \( d_{zx} \) leading to two-dimensional (2D) \( \alpha \)- and \( \beta \)-bands [Figs. 1a) and d)]. This kind of hierarchy and topology of the hybridizations can lead to a dimensional crossover between 1D and 2D dispersive behavior [5].

For our discussion we use a slave-boson technique which allows us to describe qualitatively the emergence of quasiparticles from fractionalized electrons and their inter-layer tunneling.

2. Model

Our basic model consists of two sets of 1D bands described by a Hubbard Hamiltonian including only nearest-neighbor hopping. In order to deal with the correlation effects we introduce a slave-boson approach assuming that double occupancy is strongly suppressed. Charge and spin degrees of freedom are represented by independent operators, the bosonic \( b_{\nu i}^\dagger \) (holon) and the fermionic \( f_{\nu i \sigma}^\dagger \) (spinon), respectively (\( \nu \): band index; \( i \): site index; \( \sigma \): spin index). The electron is then a composite object with the operator

\[
\begin{align*}
\mathcal{c}_{\nu i \sigma}^\dagger &= f_{\nu i \sigma}^\dagger b_{\nu i}.
\end{align*}
\]

Constraints associated with this slave-boson representation (no double occupancy) are taken into account on a global mean-field level and the hopping part of the Hamiltonian is decoupled by introducing the mean fields

\[
\begin{align*}
\chi_{\nu i}^b &= \langle b_{\nu i}^\dagger b_{\nu i} \rangle,  \\
\chi_{\nu i}^f &= \sum_{\sigma} \langle f_{\nu i \sigma}^\dagger f_{\nu i \sigma} \rangle.
\end{align*}
\]

With these approximations we arrive at a slave-boson mean-field Hamiltonian for spinons and holons in two independent 1D bands,

\[
\mathcal{H}_0 = \sum_{\nu, k, \sigma} \epsilon_{\nu k} f_{\nu k \sigma}^\dagger f_{\nu k \sigma} + \sum_{\nu, k} \omega_{\nu k} b_{\nu k}^\dagger b_{\nu k},
\]

with \( \epsilon_{\nu k} = -2t \chi^b \cos(k_i) + \lambda - \mu \) the spinon and \( \omega_{\nu k} = -2t \chi^f \cos(k_i) + \lambda \) the holon energy (\( \lambda \): Lagrange multiplier for the global constraint). This emulates effectively the spin-charge separation of the 1D correlated electron system. We now add the next-nearest-neighbor inter-orbital hopping via two O 2p-orbitals as displayed in Fig. 1d). This weaker hopping term connects the different 1D electron systems and may be written in the slave-boson representation as

\[
\mathcal{H}' = \sum_{\sigma} \sum_{k, k', q} \left( g_q f_{1k + q \sigma}^\dagger b_{1k}^\dagger b_{2k' + q \sigma} + h.c. \right),
\]
with $g_{\vec{q}} = -4t' \sin(q_x) \sin(q_y)$. Since only electrons can be transferred between chains, this invokes that a spinon and holon have to correlate to yield hopping. Thus, we may interpret $H'$ as an effective interaction term introducing attractive coupling between the two subspecies with the tendency to recombine them to an electronic quasiparticle. The electronic spectrum can now be investigated using the retarded single-electron Green’s function defined as

$$G^{\nu\nu'}(\vec{q},t) = \frac{\Theta(t)}{N^2} \left\{ \sum_{\vec{k}} h^{\dagger}_{\nu\vec{k}+\vec{q}}(t) f_{\nu\vec{k}\sigma}(t) \sum_{\vec{k}'} f^{\dagger}_{\nu'\vec{k}'+\vec{q}\sigma}(0) b_{\nu'\vec{k}'}(0) \right\},$$

where the electron operators have already been replaced by the spinon and holon operators, $N$ is the number of lattice sites and $\Theta(t)$ is the step-function.

Within RPA this Green’s function yields in energy representation

$$G^{\nu\nu'}(\vec{q},E) = \frac{G^{\nu}_{0}(\vec{q},E)}{1 - (g_{\vec{q}})^2 G^{\nu}_{0}(\vec{q},E) G^{\nu}_{0}(\vec{q},E)},$$

where

$$G^{\nu}_{0}(\vec{q},E) = \frac{1}{N^2} \sum_{\vec{k}} \frac{n^{(\nu)}_{E}(\vec{k}+\vec{q}) + n^{(\nu)}_{B}(\vec{k})}{E - \varepsilon_{\nu\vec{k}+\vec{q}} + \omega_{\nu\vec{k}}}$$

is the bare Green’s function resulting from the Hamiltonian (1) without inter-band hopping.

**3. Results**

The total spectral density in the Green’s function (4), is evaluated numerically for an electron concentration $n = 1.33$ and $t'/t = 0.15$, fitting the de Haas-van Alphen Fermi surface [6].

The spectrum is displayed in Fig. 2 where at high temperature the spectrum resembles the two-particle continuum of incoherent spinon-holon excitations [Fig. 2a)] and only at lower temperature spectral weight builds up to form two quasiparticle bands [Fig 2b)]. Within our approach the quasiparticle states remain well-defined even away from the Fermi energy because we ignore the lifetime effect due to the scattering among the quasiparticles.

The loss of spectral weight upon increasing temperature can also be seen in Figs. 1b) and c) where the $q$-dependence of the spectral weight is plotted at the Fermi energy. While for low temperatures a 2D Fermi surface is well defined by quasiparticles, the quasiparticle weight decreases and the Fermi surface fades away as the temperature is increased.

![Figure 2](image-url)
The quasiparticle weight does not arise evenly around the Fermi surface upon lowering the temperature, but as a growing arc around the [110] direction. The evolution of the length of this arc with temperature is shown in Fig. 3.

Finally, considering the c-axis transport within a tunneling approach, two regimes have to be studied separately, as the coherent weight of quasiparticles at the Fermi energy is lost completely for $T \sim 0.1t$ (cf. Fig. 1). For temperatures $T \ll 0.1t$, the main contribution to the tunneling current comes from coherent spinon-holon pairs which, however, decreases upon growing temperature due to the diminishing quasiparticle weight. This leads to a metallic temperature dependence of the resistivity. For high temperatures, i.e. $T \gg 0.1t$, coherent quasiparticles that could tunnel between layers have disappeared. Therefore, the quasiparticle picture becomes inappropriate and we have to take a different approach whereby spin and charge degrees of freedom are independent. In the tunneling process of an electron, a spinon and a holon (charge carrier) have to be transferred simultaneously giving rise to an incoherent tunneling [7]. This can be described by estimating the holon transfer probability with Fermi Golden Rule. The temperature dependence of the resistivity at high temperature is thus dominated by the spinon phase-space contribution and results in a $1/T$, i.e. an insulating behavior, in qualitative agreement with experiment [2].

4. Conclusion
In our discussion the regime change of the c-axis transport in Sr$_2$RuO$_4$ is interpreted as a dimensional crossover (from 1D to 2D) for the electronic states in the basal plane. We have shown that the slave-boson approximation can give a qualitative understanding and provides interesting insight into the change of transport properties. Our results lead to a picture where with decreasing temperature a Fermi surface appears through gradually extending arcs of finite quasiparticle weight. The difference between the metallic and insulating behavior can be understood as a change between dominant coherent to dominant incoherent tunneling due to the vanishing of coherent quasiparticles as temperature is raised.

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