Fermi-liquid versus non-Fermi-liquid behavior in a two-band model of high-temperature superconductivity

C. Castellani
Dipartimento di Fisica, Università La Sapienza, I-00185 Rome, Italy

G. Kotliar
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 19 September 1988)

We solve an extended Hubbard model describing a system with two $N$-fold degenerate bands in the limit $N = \infty$. The system exhibits a phase transition from Fermi liquid to non-Fermi liquid as the exchange interaction becomes comparable with the hybridization energy.

The discovery of high-temperature superconductivity has renewed our interest in the understanding of the possible phases of the Hubbard model. Anderson\(^1\) and co-workers have emphasized the existence of possible phases which cannot be described in terms of Fermi-liquid theory. Mean-field theory so far has been unable to reproduce this scenario except in the case where the breakdown of Fermi liquid is due to the onset of magnetic long-range order.\(^2\)

In this paper we address this question by examining a version of the two-band model currently used to study the high-temperature superconductivity in the rare-earth-based copper oxides.\(^3\)

\[
H = e_0^2 \sum_i \epsilon_{l \alpha} f_i^\dagger f_i + \frac{U}{N} \sum_{\langle i, j \rangle \alpha \sigma} d_{i \alpha}^\dagger d_{j \alpha} + \epsilon_p \sum_{i \sigma} p_{i \sigma} p_{i \sigma} + U \sum_{i \sigma \sigma'} d_{i \sigma}^\dagger d_{i \sigma} d_{i \sigma'}^\dagger d_{i \sigma'} - \frac{2t}{\sqrt{N}} \sum_{\sigma} \gamma_k (d_{k \sigma}^\dagger p_{k \sigma} + p_{k \sigma} d_{k \sigma}),
\]

(1)

in the limit of infinite $U$. $p_{i \sigma}$ are creation operators for an orbital which hybridizes with a $d_{i \sigma}$ copper orbital with a hybridization matrix element $\gamma_k$. The term proportional to $J$ in Eq. (1) represents the exchange between nearest-neighbor copper electrons generated by virtual high-energy charge fluctuations. $\sigma$ takes values from 1 to $N$, $1/N$ being the expansion parameter of the theory. The physically relevant value is $N = 2$.

In the two-band model of the copper oxide planes, as discussed by Emery and co-workers,\(^4\) the copper-oxygen exchange is given by $t_{pd}^2/(\epsilon_p - \epsilon_d^2)$ and the copper-copper superexchange is of the order of $t_{pd}^4/(\epsilon_p - \epsilon_d^2)^3$ in the limit of very large $U$. Since we scale $t_{pd}$ as $t/\sqrt{N}$ with $t$ finite, if we set $J = 0$ in Eq. (1) the copper-copper superexchange would appear as a $1/N^2$ effect. For $N = 2$, the estimates of Ref. 3 indicate $J \sim 0.2$ eV, $t \sim 0.7$ eV, $\epsilon_p - \epsilon_d \sim 1 - 2$ eV. Therefore, the copper-copper superexchange is smaller but of the same order of magnitude as the copper-oxygen exchange. Here we propose to introduce the superexchange explicitly in the Hamiltonian and to scale the exchange constant as $J/N$.

For $J = 0$, this model was studied in Ref. 4 where it was pointed out that the $N = \infty$ theory exhibits a Brinkman-Rice transition at a finite value of the coupling $t^2/(\epsilon_p - \epsilon_d)^2$. For $\delta = 0$ this model was considered by Affleck and Marston\(^5\) who showed that the model exhibits several magnetic phases without spin long-range order: the flux phase, the uniform phase, and the dimer phase.

To study the $N = \infty$ limit, it is convenient to use a functional integral representation of the model. The partition function of the model is given by

\[
Z = \int d\epsilon_0 d\epsilon_1 db_1 db_2 db_3 d\epsilon d\epsilon d\epsilon \exp \left[ -\int_0^\beta S \right],
\]

\[
S = \frac{N}{\beta} \sum_{\langle i, j \rangle} \Delta_{ij}^2 - \sum_i \lambda_i (b_i^\dagger b_i - Q) - \sum_i p_{i \alpha} \left( \theta / \theta \right) - \epsilon_p + \mu) p_{i \alpha} + d_{i \alpha}^\dagger \left( \theta / \theta \right) - \epsilon_d - \mu + \sum_{\langle i, j \rangle} \Delta_{ij} d_{i \alpha}^\dagger d_{j \alpha} + \Delta_{ij}^2 d_{i \alpha}^\dagger d_{j \alpha} - \frac{2it}{\sqrt{N}} \sum_{k \sigma} \gamma_k (p_{k \sigma} d_{k \sigma} - q_0 p_{k \sigma} + d_{k \sigma}^\dagger q_0 p_{k \sigma}).
\]

(2)

Following Refs. 4, 6, and 7, we have replaced the $U = \infty$ limit by adding a Bose degree of freedom $b_i^\dagger$ to label the empty site. The constraint on the occupancy of copper sites

\[
b_i^\dagger b_i + \sum_{\alpha} d_{i \alpha}^\dagger d_{i \alpha} = Q = qN
\]

(3)

is then enforced by the Lagrange multiplier $\lambda_i$ multiplying the constraint (3). Originally $q = 1/N$, but here it is taken to be an independent parameter to generate a controlled loop expansion.\(^6\) The exchange term is decoupled using a field $\Delta_{ij}$. Integrating out the Fermi fields one obtains an effective action for the Bose fields.
The $N=\infty$ limit is dominated by a saddle point which is taken to be static. It is determined from the extremum of the mean-field free energy. $F_{\text{mf}}$ expressed in terms of $(\Delta d_{ij}), (\beta d_{ij}) = \sqrt{N} r$ and $(\lambda d_{ij}) = \lambda$. The possible saddle points for the field $\Delta d_{ij}$ were discussed by Affleck and Marston.\textsuperscript{5} Besides the uniform phase which can be shown to be unstable in different ways they considered (a) the dimer phase $(d_{i}^{+} d_{i-\Delta}^{\dagger}) = \Delta$, $(d_{i}^{+} d_{i+\Delta}^{\dagger}) = (d_{i} d_{i+\Delta}) = (d_{i} d_{i-\Delta}) = 0$; and (b) the flux phase $(d_{i}^{+} d_{i-\Delta}^{\dagger}) = \Delta$, $(d_{i}^{+} d_{i+\Delta}^{\dagger}) = (d_{i} d_{i+\Delta}) = (d_{i} d_{i-\Delta}) = i \Delta$. $i$ is an even copper sublattice site and $i \pm x, i \pm y$ denote the nearest site to the right, left, above, and below site $i$.

The mean-field free energy per copper site $N_s$ is written as

$$F = \frac{1}{J} \frac{\Delta^2}{2} - \lambda (r^2 - q) - \frac{1}{N_s} \sum_{k, \alpha, \beta} T \ln \left[ 1 + \exp \left( - \frac{E_{\beta}^d + \mu}{T} \right) \right], \quad (4)$$

where $E_{\beta}^d$ are the eigenvalues of the matrix

$$\begin{pmatrix}
2\Delta \cos k_x + (\epsilon_0 - \lambda) & -2i \Delta \cos k_y & -2r \gamma_k \\
-2i \Delta \cos k_y & 2\Delta \cos k_x + (\epsilon_0 - \lambda) & 0 \\
-2r \gamma_k & 0 & \epsilon_0 \\
0 & -2r \gamma_k + G & 0
\end{pmatrix}$$

in the dimer phase. $k$ varies in the reduced Brillouin zone and $G=(\pi, \pi)$ has been introduced to take care of the doubling of unit cell.

The flux-phase free energy is written as

$$F = \frac{1}{J} 2\Delta^2 - \lambda (r^2 - q) - \frac{1}{N_s} \sum_{k, \alpha, \beta} T \ln \left[ 1 + \exp \left( - \frac{E_{\beta}^d + \mu}{T} \right) \right], \quad (6)$$

with $E_{\beta}^d$ eigenvalues of

$$\begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & \epsilon_0 \\
\epsilon_0 & -2r \gamma_k + G & 0
\end{pmatrix}$$

with the obvious notation $f_{k_{1,2}^\pm} = f(E_{k_{1,2}^\pm} - \mu)$, $f$ being the Fermi function,

$$R_{k_{1,2}} = [(\epsilon_0^d - \epsilon_0^d)^2 + 16r^2 t^2 \gamma_k^2]^{1/2}$$

and

$$u_{k_{1,2}} = \frac{1}{2} \left[ 1 + \frac{\epsilon_0^d - \epsilon_0^d(k)}{R_{k_{1,2}}} \right],$$

$$v_{k_{1,2}} = \frac{1}{2} \left[ 1 - \frac{\epsilon_0^d - \epsilon_0^d(k)}{R_{k_{1,2}}} \right].$$

Equation (14) states that the total number of holes is given by $N_q(1+\delta)$. From now on we shall assume $q = \frac{1}{2}$, so that $\delta$ is the doping with respect to one hole per copper site.

There are two different physical situations. $r\neq0$ corresponds to hybridization between $p-d$ bands and to a non-vanishing quasiparticle residue in the single-particle Green’s function (Fermi-liquid phase). At $r=0$, this picture breaks down and both hybridization and quasiparticle residue are zero (non-Fermi-liquid phase).

We study how these transitions occur by solving Eqs. (11)–(13) in the zero-temperature limit, for small $\delta$ and well in the insulating side of the Mott transition, i.e., $t/(\epsilon_0^d - \epsilon_0^d) \ll 1$. We will also assume $t/J \gg 1$. In this regime $\Delta$ can be approximated by the $\delta=0$ solution of Eq. (11): $\Delta = \frac{1}{2} J$ in the dimer phase and $\Delta = 0.239 J$ in the flux phase.
Combining Eqs. (12) and (14) we find
\[
g_{\delta} + r^{2} = \frac{1}{N_{k}} \sum_{k} (1 - u_{k}^{2}) f_{\pm k}^{-}\nabla_{k} + (1 - u_{\pm k}^{2}) f_{\pm k}^{-} + u_{k}^{2} f_{\pm k}^{+} + u_{\pm k}^{2} f_{\pm k}^{+},
\]
which can be solved for \( r \) vs \( \varepsilon_{p} - \varepsilon_{d}^{0} \). In the dimer case we obtain
\[
r^{2} = \delta g \left[ \frac{a_{1}}{(\varepsilon_{p} - \varepsilon_{d})^{2}} + \frac{a_{2}}{(\varepsilon_{p} - \varepsilon_{d}^{0})^{2}} \right],
\]
with \( a_{1,2} = 4(1/N_{k}) \sum_{k} \gamma_{k} f_{\pm k}^{-} \) for \( \varepsilon_{p} - \varepsilon_{d} > 0 \) and \( r^{2}/(\varepsilon_{p} - \varepsilon_{d})^{2} \ll 1 \), while
\[
r^{2} = \frac{2\delta g \Delta}{a_{1} \Delta^{2}},
\]
when \( \varepsilon_{p} - \varepsilon_{d}^{0} = 0 \).

When \( \varepsilon_{p} - \varepsilon_{d} > 0 \) the only solution is \( r = 0 \), \( \varepsilon_{p} \) and, therefore, \( \varepsilon_{d} \) and \( \varepsilon_{d}^{0} \), is determined from Eq. (13). When \( J \ll r^{2}/(\varepsilon_{p} - \varepsilon_{d}^{0}) \), \( \varepsilon_{d} \approx \varepsilon_{d}^{0} \approx \varepsilon_{p} - c_{1} J^{2}/(\varepsilon_{p} - \varepsilon_{d}^{0}) \). As \( J \) increases, \( \varepsilon_{p} - \varepsilon_{d}^{0} \) decreases. For sufficiently large \( J \), Eq. (13) with \( r \neq 0 \) becomes inconsistent with Eq. (15) and \( r \) jumps discontinuously to zero. This occurs first when
\[
\varepsilon_{p} = \frac{\varepsilon_{d}^{0} - \Delta}{4} = 4c_{2} \frac{t^{2}}{J},
\]
and \( c_{2} = (1/N_{k}) \sum \gamma_{k} f_{\pm k}^{-} \) in the limit of vanishing \( \delta \).

This first-order transition can be understood in simple physical terms. In the Fermi-liquid regime we gain hybridization energy \( t^{2}/(\varepsilon_{p} - \varepsilon_{d}^{0}) \) per hole but we lose exchange energy \( J \) per hole. When \( J \) is large it becomes advantageous to occupy only the lowest dimerized band and to put the additional holes in the \( p \) band.

In the flux case, for small \( \delta \), only the regions in \( k \) space around \((\pm \pi/2, \pm \pi/2)\) are important and we approximate them by a linear dispersion of the \( d \) bands and approximate \( y_{k} \) by \( y_{k}(\pi/2, \pi/2) \equiv y \). With these approximations and \( q = \frac{1}{2} \), Eqs. (13)–(15) become
\[
\frac{1}{2} \delta + r^{2} = \int_{-j}^{\infty} \frac{dx}{J^{2}} \left[ 1 - \frac{\varepsilon_{p} - \varepsilon_{d} - x}{(\varepsilon_{p} - \varepsilon_{d} - x)^{2} + 4y^{2}t^{2}r^{2} J} \right],
\]
\[
\varepsilon_{d} - \varepsilon_{d}^{0} = \int_{-j}^{\infty} \frac{dx}{J^{2}} \left[ 1 - \frac{4y^{2}t^{2}}{(\varepsilon_{p} - \varepsilon_{d} - x)^{2} + 4y^{2}t^{2}J} \right],
\]
with \( \varepsilon_{d} = \varepsilon_{d}^{0} - \Delta \). The energy \( \varepsilon_{d} \) is defined by Eq. (20). For \( \varepsilon_{p} - \varepsilon_{d} > 0 \) Eq. (18) is solved by
\[
r^{2} = \frac{\delta}{2} \int_{-j}^{\infty} dx \frac{1}{J^{2}} \left[ \frac{1}{(\varepsilon_{p} - \varepsilon_{d} - x)^{2} + 4y^{2}t^{2}J} \right],
\]
which can be solved to give \( r^{2} = (\varepsilon_{p} - \varepsilon_{d})^{2}/8y^{2}t^{2}J \).

That is, \( r^{2} \) vanishes as \( \varepsilon_{d} \) approaches \( \varepsilon_{p} \). The second equation can be solved for \( \varepsilon_{d} \). As the ratio \( t^{2}/(\varepsilon_{p} - \varepsilon_{d})^{2} \) increases \( \varepsilon_{p} - \varepsilon_{d} \) decreases and eventually vanishes when
\[
(\varepsilon_{p} - \varepsilon_{d})^{2} = \frac{4y^{2}t^{2}}{J} (\varepsilon_{d}^{0} + J).
\]

At this coupling the system undergoes a continuous transition to a non-Fermi-liquid phase. The same criteria are obtained by examining the stability of the non-Fermi-liquid solution at \( r^{2} = 0 \).

In conclusion, we presented a model which can be solved in a \( 1/N \) expansion and which exhibits a Brinkman-Rice transition at a finite density of holes. It is significant that close to this phase transition the effective mass and the susceptibility remain finite while the quasiparticle residue becomes vanishingly small. Since the thermodynamical properties of the high-temperature superconductors are rather normal while its transport properties are very anomalous, it is tempting to associate this strange behavior with the proximity to the transition line found in this paper. It is clearly of interest to compute the change energy \( J \) per hole. When \( J \) is large it becomes advantageous to occupy only the lowest dimerized band and to put the additional holes in the \( p \) band.

1/N corrections around the saddle point and to map our phase diagram with a realistic copper oxygen band structure. This task will be carried out in a future publication. It is not obvious how to generalize this work to the infinite \( U \) one-band Hubbard model. The difficulty seems to be that in this case the slave-boson expectation value measures both the number of carriers and the amount of Fermi-liquid coherence, and, therefore, can never vanish away from half filling at mean-field level. In the two-band model these two roles are somewhat decoupled by the extra degree of freedom provided by the additional band.

In this paper we focused on the transition between the Fermi-liquid state and a non-Fermi-liquid state which takes place when the exchange energy \( J \) becomes comparable to the hybridization energy \( t^{2}/(\varepsilon_{p} - \varepsilon_{d}^{0}) \). This transition was studied analytically using the mean-field technique and an expansion valid for small density of holes. This transition is different from the first-order phase transition between the dimerized phase and the metallic phase with uniform \( \Delta \) that one encounters when one increases the hole concentration \( \delta \) and the renormalized kinetic energy \( \delta t^{2}/(\varepsilon_{p} - \varepsilon_{d}^{0}) \) becomes larger than the exchange \( J \). This transition has a one-band analog and has been studied in Ref. 5.
One of us (G.K.) would like to thank the condensed matter physics group at the University of Rome where this collaboration began for their hospitality. This work is supported by the National Science Foundation under Grants No. DRM-85-21377 and No. DMR-86-57557. The authors (C.C. and G.K.) would like to acknowledge the hospitality of the International Center for Theoretical Physics at Trieste, where part of this research was carried out.

8Equation (15) admits also a nonperturbative solution with a higher value $r \gg \delta$ which, however, does not play any role in our context because Eq. (13) obliged $r$ to be small.
9The stability of the magnetically correlated $d$ band with respect to hybridization was also found in a different context (three-band model) by C. Castellani, C. Di Castro, and M. Grilli, Physica C 153-155, 1659 (1988).