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

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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]

$$H=\varepsilon_d^0\sum_i f_{i\sigma}^\dagger f_{i\sigma}+\frac{J}{N}\sum_{(i,j)\sigma\sigma'} d_{i\sigma}^\dagger d_{i\sigma'} d_{j\sigma'}^\dagger d_{j\sigma}+\varepsilon_p\sum_{i,\sigma} p_{i\sigma}^\dagger p_{i\sigma}+U\sum_{i,\sigma\neq\sigma'} d_{i\sigma}^\dagger d_{i\sigma} d_{i\sigma'}^\dagger d_{i\sigma'}-\frac{2t}{\sqrt{N}}\sum_\sigma \gamma_k (d_{k\sigma}^\dagger p_{k\sigma}+p_{k\sigma}^\dagger d_{k\sigma}) , \quad (1)$$

in the limit of infinite U. $p_{\sigma i}$ are creation operators for an oxygen orbital which hybridizes with a $d_{\sigma i}^\dagger$ copper orbital with a hybridization matrix element γ_k. The term proportional to J in Eq. (1) represents the exchange between nearest-neighbor copper electrons generated by virtual high-energy charge fluctuations. σ 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,[3] the copper-oxygen exchange is given by $t_{pd}^2/(\varepsilon_p-\varepsilon_d^0)$ and the copper-copper superexchange is of the order of $t_{pd}^4/(\varepsilon_p-\varepsilon_d^0)^3$ 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, and $\varepsilon_p-\varepsilon_d\sim 1$–$2$ 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 $t^2/(\varepsilon_p-\varepsilon_d)^2$. 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

$$Z=\int d\lambda db^\dagger dbdd_\sigma^\dagger dd_\sigma dp_\sigma^\dagger dp_\sigma d\Delta^\dagger d\Delta \exp\left(-\int_0^\beta S\right),$$

$$S=\frac{N}{J}\sum_{(i,j)}\Delta_{ij}^*\Delta_{ij}-\sum_i\lambda_i(b_i^\dagger b_i-Q)-\sum_{i,\sigma}p_{i\sigma}^\dagger[(\partial/\partial\tau)-(\varepsilon_p-\mu)]p_{i\sigma}+d_{i\sigma}^\dagger[(\partial/\partial\tau)-(\varepsilon_d-\mu)+\lambda_i]d_{i\sigma}$$
$$+\sum_{(i,j),\sigma}\Delta_{ij}d_{i\sigma}^\dagger d_{j\sigma}+\Delta_{ij}^* d_{j\sigma}^\dagger d_{i\sigma}-\frac{2t}{\sqrt{N}}\sum_{k,q,\sigma}\gamma_k(p_{k\sigma}^\dagger b_q^\dagger d_{k+q\sigma}+d_{k+q\sigma}^\dagger b_q p_{k\sigma}) . \quad (2)$$

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

$$b_i^\dagger b_i+\sum_\sigma d_{\sigma i}^\dagger d_{\sigma i}=Q=qN \quad (3)$$

is then enforced by the Lagrange multiplier λ_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.[6,7] The exchange term is decoupled using a field Δ_{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. $F_{\rm mf}$ expressed in terms of $\langle\Delta_{ij}\rangle$, $\langle b_i\rangle=\sqrt{N}r$ and $\langle\lambda_i\rangle=\lambda$. The possible saddle points for the field Δ_{ij} were discussed by Affleck and Marston.[5] Besides the uniform phase which can be shown to be unstable in different ways they considered (a) the dimer phase $\langle d_i^\dagger d_{i-x}\rangle=\Delta$, $\langle d_i^\dagger d_{i+x}\rangle=\langle d_i^\dagger d_{i+y}\rangle=\langle d_i^\dagger d_{i-y}\rangle=0$; and (b) the flux phase $\langle d_i^\dagger d_{i+x}\rangle=\langle d_i^\dagger d_{i-x}\rangle=\Delta$, $\langle d_i^\dagger d_{i+y}\rangle=\langle d_i^\dagger d_{i-y}\rangle=i\Delta$. 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

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

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

$$\begin{pmatrix} \varepsilon_d^0-\lambda+\Delta\cos k_x & -i\Delta\sin k_x & -2rt\gamma_k & 0 \\ i\Delta\sin k_x & \varepsilon_d^0-\lambda-\Delta\cos k_x & 0 & -2rt\gamma_{k+G} \\ -2rt\gamma_k & 0 & \varepsilon_p & 0 \\ 0 & -2rt\gamma_{k+G} & 0 & \varepsilon_p \end{pmatrix} \tag{5}$$

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

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

with $E_{k\beta}^{\alpha}$ eigenvalues of

$$\begin{pmatrix} 2\Delta\cos k_x+(\varepsilon_d^0-\lambda) & -2i\Delta\cos k_y & -2rt\gamma_k & 0 \\ 2i\Delta\cos k_y & -2\Delta\cos k_x+(\varepsilon_d^0-\lambda) & 0 & -2rt\gamma_{k+G} \\ -2rt\gamma_k & 0 & \varepsilon_p & 0 \\ 0 & -2rt\gamma_{k+G} & 0 & \varepsilon_p \end{pmatrix}. \tag{7}$$

The free energies (4) and (6) can be in principle extremized numerically with a realistic band-structure dispersion γ_k. Here we will make some drastic simplification as to the form of γ_k in order to gain insight into the problem. If we assume $\gamma_k=\gamma_{k+G}$ the problem simplifies and we find the following eigenvalues:

$$E_{k\frac{1}{2}}^{\mp}=\tfrac{1}{2}\{(\varepsilon_{dk\frac{1}{2}}+\varepsilon_p)\pm[(\varepsilon_{dk\frac{1}{2}}-\varepsilon_p)^2+16r^2t^2\gamma_k^2]^{1/2}\} \tag{8}$$

with

$$\varepsilon_{dk\frac{1}{2}}=\varepsilon_d^0-\lambda\mp\Delta \tag{9}$$

the energy of the exchange renormalized d subband if we assume dimer order, and

$$\varepsilon_{dk\frac{1}{2}}=\varepsilon_d^0-\lambda\mp 2\Delta(\cos^2k_x+\cos^2k_y)^{1/2} \tag{10}$$

assuming flux order. Differentiating (4) and (6), we obtain the mean-field equations

$$\frac{\Delta}{J}=\frac{1}{N_s}\sum_k K(k)(u_{k1}^2f_{k1}^-+v_{k1}^2f_{k1}^+-u_{k2}^2f_{k2}^--v_{k2}^2f_{k2}^+), \tag{11}$$

$$r^2+\frac{1}{N_s}\sum_k(u_{k1}^2f_{k1}^-+u_{k2}^2f_{k2}^-+v_{k1}^2f_{k1}^++v_{k2}^2f_{k2}^+)=q, \tag{12}$$

$$-\lambda r=\frac{1}{N_s}\sum_k 4rt^2\gamma_k^2\left(\frac{f_{k1}^-+f_{k2}^-}{R_{k1}}-\frac{f_{k1}^++f_{k2}^+}{R_{k2}}\right), \tag{13}$$

$$q(1+\delta)\frac{1}{N_s}\sum_k(f_{k1}^-+f_{k2}^-+f_{k1}^++f_{k2}^+), \tag{14}$$

with the obvious notation $f_{k1,2}^{\mp}=f(E_{k1,2}^{\mp}-\mu)$, f being the Fermi function,

$$R_{k1,2}=[(\varepsilon_{dk}^{1,2}-\varepsilon_p)^2+16r^2t^2\gamma_k^2]^{1/2}$$

and

$$u_{k1,2}^2=\frac{1}{2}\left(1+\frac{\varepsilon_p-\varepsilon_d^{1,2}(k)}{R_{k1,2}}\right),$$

$$v_{k1,2}^2=\frac{1}{2}\left(1-\frac{\varepsilon_p-\varepsilon_d^{1,2}(k)}{R_{k1,2}}\right).$$

$K(k)=1$ in the dimer phase and $K(k)=\frac{1}{2}(\cos^2k_x+\cos^2k_y)^{1/2}$ in the flux phase.

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

There are two different physical situations. $r\neq 0$ corresponds to hybridization between p-d bands and to a nonvanishing 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 δ and well in the insulating side of the Mott transition, i.e., $t/(\varepsilon_p-\varepsilon_d^0)\ll 1$. We will also assume $t/J\gg 1$. In this regime Δ can be approximated by the $\delta=0$ solution of Eq. (11): $\Delta=\frac{1}{2}J$ in the dimer phase and $\Delta\simeq 0.239J$ in the flux phase.

Combining Eqs. (12) and (14) we find

$$q\delta+r^2=\frac{1}{N_s}\sum_k(1-u_{k1}^2)f_{k1}^- + (1-u_{k2}^2)f_{k2}^- + u_{k1}^2 f_{k1}^+ + u_{k2}^2 f_{k2}^+ , \quad (15)$$

which can be solved for r vs $\varepsilon_p-\varepsilon_d^0$. In the dimer case we obtain

$$r^2=\delta q\Big/\left[\alpha_1\frac{t^2}{(\varepsilon_p-\varepsilon_{d1})^2}+\alpha_2\frac{t^2}{(\varepsilon_p-\varepsilon_{d2})^2}\right], \quad (16)$$

with $\alpha_{1,2}=4(1/N_s)\sum_k\gamma_k^2 f_{k_{1,2}}^-$ for $\varepsilon_p-\varepsilon_{d2}>0$ and $r^2t^2/[(\varepsilon_p-\varepsilon_{d2})^2]\ll 1$, while

$$r^2=\frac{2\delta q\Delta^2}{\alpha_1 t^2}, \quad (17)$$

when $\varepsilon_p-\varepsilon_{d2}\to 0$.

When $\varepsilon_p-\varepsilon_{d2}<0$ the only solution is $r=0$.[8] λ and, therefore, ε_{d1} and ε_{d2}, is determined from Eq. (13). When $J\ll t^2/(\varepsilon_p-\varepsilon_d^0)$, $\varepsilon_{d1}\cong\varepsilon_{d2}\cong\varepsilon_p-c_1t^2/(\varepsilon_p-\varepsilon_d^0)$.[4] As J increases, $\varepsilon_p-\varepsilon_{d2}$ 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

$$(\varepsilon_p-\varepsilon_d^0-\Delta)\cong 4c_2\frac{t^2}{J},$$

and $c_2=(1/N_s)\sum\gamma_k^2 f_{k1}^-$ in the limit of vanishing δ.

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.[9]

In the flux case, for small δ, 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 γ_k by $\gamma_k(\pi/2,\pi/2)\equiv\gamma$. With these approximations and $q=\frac{1}{2}$, Eqs. (13)–(15) become

$$\tfrac{1}{2}\delta+r^2=\int_{-J}^{\varepsilon_0}\frac{dx\,|x|}{2J^2}\times\left[1-\frac{(\varepsilon_p-\varepsilon_d-x)}{[(\varepsilon_p-\varepsilon_d-x)^2+16\gamma^2t^2r^2]^{1/2}}\right], \quad (18)$$

$$\varepsilon_d-\varepsilon_d^0=\int_{-J}^{\varepsilon_0}\frac{dx\,|x|}{J^2}\frac{4\gamma^2t^2}{[(\varepsilon_p-\varepsilon_d-x)^2+16\gamma^2t^2r^2]^{1/2}}, \quad (19)$$

$$\tfrac{1}{2}(1+\delta)=\int_{-J}^{\varepsilon_0}\frac{dx\,|x|}{J^2}, \quad (20)$$

with $\varepsilon_d=\varepsilon_d^0-\lambda$. The energy ε_0 is defined by Eq. (20). For $\varepsilon_p-\varepsilon_d>\varepsilon_0$ Eq. (18) is solved by

$$r^2=\delta/2\int_{-J}^{\varepsilon_0}dx\left(\frac{|x|\gamma^2t^2 4}{(\varepsilon_p-\varepsilon_d-x)^2}-1\right). \quad (21)$$

When $\varepsilon_p-\varepsilon_d<\varepsilon_0$ we have $y=(\varepsilon_p-\varepsilon_d)^2/J^2$ holes in the upper d band and $\delta-y$ holes in the p band. It is convenient to rewrite Eq. (18) in terms of the variable y

$$r^2+\tfrac{1}{2}y=\int_{-J}^{\varepsilon_p-\varepsilon_d}\frac{dx\,|x|}{2J^2}\left[1-\frac{(\varepsilon_p-\varepsilon_d-x)}{[(\varepsilon_p-\varepsilon_d-x)^2+16\gamma^2t^2r^2]^{1/2}}\right]-\int_{\varepsilon_p-\varepsilon_d}^{\varepsilon_0}\frac{dx\,|x|}{2J^2}\left[1-\frac{(x+\varepsilon_d-\varepsilon_p)}{[(\varepsilon_p-\varepsilon_d-x)^2+16\gamma^2t^2r^2]^{1/2}}\right], \quad (22)$$

which can be solved to give $r^2=(\varepsilon_p-\varepsilon_d)^2/8\gamma^2t^2\ln J/\varepsilon^0$. That is, r^2 vanishes as ε_d approaches ε_p. The second equation can be solved for $(\varepsilon_p-\varepsilon_d)$. As the ratio $tJ/(\varepsilon_p-\varepsilon_d^0)^2$ increases $\varepsilon_p-\varepsilon_d$ decreases and eventually vanishes when

$$(\varepsilon_p-\varepsilon_d^0)=\frac{4\gamma^2t^2}{J^2}(\varepsilon_0+J). \quad (23)$$

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 $1/N$ 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 Δ that one encounters when one increases the hole concentration δ 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.

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