

- 14) E. Takayama-Muromachi et al.: J. Appl. Phys. 27, L223 (1988).
H. Kamimura et al.: Solid State Comm. 67, 363 (1988).
A. Bianconi et al.: preprint.
- 15) P.W. Anderson: Science 235, 1196 (1987).
G. Baskaran, Z. Zou and P.W. Anderson: Solid State Commn. 63, 973 (1987).
- 16) to be published.
- 17) P.B. Wiegmann: Phys. Rev. Lett. 60, 821 (1988).
- 18) B.I. Shraiman and E.D. Siggia: Phys. Rev. Lett. 61, 467(1988).
- 19) V.J. Emery and G. Reiter: preprint.
- 20) A. Aharony et al.: Phys. Rev. Lett. 60, 1330 (1988).
- 21) N. Nagaosa, Y. Hatsugai and M. Imada: submitted to J. Phys. Soc. Jpn.
- 22) H. Yokoyama and H. Shiba: J. Phys. Soc. Jpn. 57, 2482 (1988).

Fermi Liquid and Non Fermi Liquid Phases of the Extended Hubbard Model

G. Kotliar

Massachusetts Institute of Technology, Cambridge, MA 02139, USA

We outline the auxiliary boson approach to the one band and two band Hubbard model. In this framework we find Fermi Liquid and Non Fermi Liquid behavior in different regions of the phase diagram. Differences and similarities with the heavy Fermion problem are emphasized.

The discovery of high temperature superconductivity¹ has led to an intensive experimental investigation of the physical properties of the rare earth based copper oxides. While there are many theoretical proposals as to the mechanism of the superconductivity, there is not yet consensus in how to model their normal and superconducting phase. In this talk I will summarize some aspects of the auxiliary boson² approach to this problem. The rationale for this approach is the belief that the copper oxides are strongly correlated systems and that the proximity to metal insulator transition is an essential feature that the ultimate theory of the copper oxides should contain. The auxiliary boson technique provides a coherent framework for addressing the strong correlation problem and has been very useful in understanding many aspects of the heavy fermion systems.³ Modelling the heavy fermions and the high temperature superconductors with the same Hamiltonian and the same technique gives us some clues of what are the essential differences, and similarities between these two systems.

The starting point of the investigation is Anderson's⁴ observation that the magnetic state of the insulating parent of the high temperature superconductor is a spin liquid with a wave function:

$$|\Phi\rangle = P \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} d_{\mathbf{k}\uparrow}^{\dagger} d_{\mathbf{k}\downarrow}^{\dagger}) |0\rangle \quad (1)$$

which resembles the projection of a BCS state with Bogolubov coefficients $u_{\mathbf{k}}, v_{\mathbf{k}} = 1/2(1 \pm E_{\mathbf{k}}/E_{\mathbf{k}})$; $E_{\mathbf{k}} = \sqrt{e_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$, and gap parameter $\Delta_{\mathbf{k}}$. $d_{\mathbf{k}\sigma}^{\dagger}$ are copper creation operators. At half filling this wave function describes a Fermi Liquid or a superconductor whose charge degrees of freedom have been totally eliminated. The excitation spin spectrum relative to that state is that of particle hole pairs with quasiparticle dispersion $E_{\mathbf{k}}$. Upon doping a small amount of charge fluctuations of the order of the doping δ is allowed and the state smoothly evolves into a superconducting state.⁴ Variational wave functions describing liquids with strongly suppressed charge fluctuations are well known in the context of the heavy fermion problem. In fact most of our current understanding of this problem is based on approximate ground states of the form⁵

$$|\psi\rangle = PG \prod_{\mathbf{k}\sigma} [u_{\mathbf{k}} + v_{\mathbf{k}} d_{\mathbf{k}\sigma}^\dagger] \prod_{\mathbf{k} < \mathbf{k}_F} p_{\mathbf{k}\sigma}^\dagger |0\rangle \quad (2)$$

where $p_{\mathbf{k}\sigma}^\dagger$, $d_{\mathbf{k}\sigma}^\dagger$ are creation operators of conduction electrons and localized electrons respectively. The Gutzwiller projection acts to eliminate the doubly occupancy of localized electrons.

Very shortly after Anderson's proposal it was established that at $\delta = 0$ the ground state of the Heisenberg model⁶ and of the insulating parents of the high temperature superconductors⁷ has antiferromagnetic long range order. I take the view that in the regime of doping where the copper oxides do not exhibit magnetic long range order they can be thought of as superconductors or fermi liquids whose charge fluctuations are strongly suppressed. From this point of view the origin of high temperature superconductivity is the proximity to the metal insulator transition which renormalizes the kinetic energy to a value small or comparable with the pairing energies. In this regime of strong correlation high temperature superconductivity is possible. At the same time the presence of strong correlations imply the existence of other competing ground states with different forms of long range order, like antiferromagnetism and dimerization, and a small but finite doping, is necessary to eliminate these instabilities.

The study of Gutzwiller projected wave functions is closely related to the auxiliary boson description of strongly correlated systems. The mean field approach to the large U Hubbard model starts with the Hamiltonian:

$$\begin{aligned} H = & -t \sum_{\langle ij \rangle, \sigma} (d_{i, \sigma}^\dagger b_j^\dagger d_{j, \sigma} + d_{j, \sigma}^\dagger b_j b_i^\dagger d_{i, \sigma}) - \mu_0 \sum_{i, \sigma} d_{i, \sigma}^\dagger d_{i, \sigma} \\ & + J \sum_{\langle ij \rangle} (\sigma_i \cdot \sigma_j - (1 - b_i^\dagger b_j)(1 - b_j^\dagger b_i)) \\ & + \sum_i \lambda_i (\sum_{\sigma} d_{i, \sigma}^\dagger d_{i, \sigma} + b_i^\dagger b_i - 1) \end{aligned} \quad (3)$$

with b_j a slave boson which ensures the single occupancy constraint on each site and $\sigma_i^a = d_{i\sigma}^\dagger \sigma_i^a d_{i\sigma}$ the copper spin operator. Mean field theory is done by performing a consistent Hartree Fock Bogolubov factorization of this Hamiltonian.⁸ This factorization respects the global SU(2) symmetry of the half filled system. The order parameters are

$$b_i = \langle b_i \rangle, \quad \Delta_{ij} = \langle d_{i\sigma}^\dagger d_{j-\sigma}^\dagger \rangle, \quad \chi_{ij} = \langle d_{i\sigma}^\dagger d_{i\sigma} \rangle. \quad (4)$$

The first solutions of the mean field equations are due to Bascaran Zou and Anderson⁹ who found, at half filling, an excitation spectrum of the form

$$E_{\mathbf{k}} = |\cos k_x + \cos k_y| \quad (5)$$

which vanishes along lines in the two dimensional Brillouin zone called the pseudofermi surface. Later Kotliar¹⁰ and Affleck and Marston¹⁰ found a lower energy phase with an excitation spectrum of particle hole pairs with a quasiparticle dispersion relation

$$E_{\mathbf{k}} = \sqrt{\cos^2 k_x + \cos^2 k_y} \quad (6)$$

vanishing on 4 Fermi points in the Brillouin zone. This $s + id$, or flux phase has an intrinsically generated flux of per plaquette. Finally there is a spin Peirls phase in which the ground state is a valence bond state and the excitations are localized and fully gapped. The SU(2) symmetry¹⁰ results in an infinite number of degenerate ground states which can be classified by their flux. Kotliar and Liu⁸ addressed the question of which spin liquid phases can be continued upon doping into superconductors. In the framework of mean field theory they found the uniform state evolves into a fermi liquid upon doping while the states with flux per plaquette like the $s + id$ phase evolve upon doping into a strongly coupled d wave superconductor with a gap function proportional to $\Delta_{\mathbf{k}} = \cos k_x - \cos k_y$. As the doping increases the ground state and the mean field equations from which it is derived evolve into a conventional weakly coupled d wave BCS superconductor.

In the slave Boson technique the physical copper electron creation operator is represented by the product

$$d_{i, \text{phys}}^\dagger = d_{i, \text{fermi}}^\dagger b_i \quad (7)$$

therefore the physical pairing order parameter decomposes into a product

$$\langle d_{i, \text{phys}}^\dagger d_{j, \text{phys}}^\dagger \rangle = \langle b_i b_j \rangle = \Delta_{\text{phys } ij}. \quad (8)$$

Hence, in this approach there are two characteristic temperatures, the critical temperature of bose condensation T_{cb} , below which $\langle b_i b_j \rangle \neq 0$ which can be thought of as a Kondo temperature signaling the onset of coherence, and T_{cRVB} , the pairing temperature below which $\langle d_{i\sigma}^\dagger d_{j-\sigma}^\dagger \rangle \neq 0$. In Fig.(1) we show a calculation of the critical temperatures using mean field theory and assuming a weak interlayer coupling to stabilize the Bose condensation. The approach to calculate $T_c(b)$ is very primitive and the consistent incorporation of finite temperature effects in the strong correlation problem remains one of the important unsolved problems in this field. In particular, there are reasons to believe that the mean field theory overestimates the slope of the curve $T_c(b)$ vs. δ . Very close to half filling the mean field solutions found are unstable against antiferromagnetism and dimerization but this is not indicated in the phase diagram.

b plays the role of quasiparticle residue and it is non zero in the normal metallic and superconducting phases. When the quasiparticle residue b is non vanishing, Δ measures the quasiparticle pairing and is proportional to the usual superconducting order parameter. As the doping increases the renormalized fermi energy increases relative to the pairing energies and the

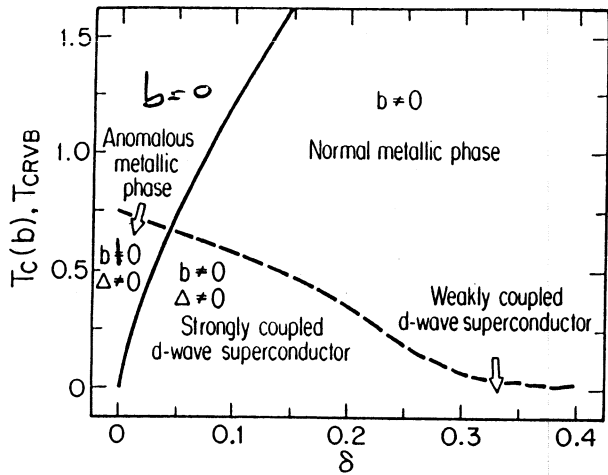


Fig 1. T_b (dot-dashed line) and T_{rvb} (dotted line) in units of J vs. filling factor. From the mean field solutions of Hamiltonian³ for $t = 10J$.

superconducting state evolves continuously into a conventional weakly coupled d wave superconductor. The phase with $b = 0$ $\Delta \neq 0$ is an anomalous non Fermi Liquid phase where there are no quasiparticles or metallic coherence since $b = 0$ $\Delta \neq 0$ indicating that pairs are present but for the system to be superconducting coherence between the pairs needs to be established. This occurs below $T_c(b)$.

The same techniques can be used to study the two band model that treats explicitly copper and oxygen holes with creation operators $d^\dagger_{\sigma i}$, $p^\dagger_{\sigma i}$ respectively. Here we generalize the spin index to run from 1 to N , $N = 2$ being the spin 1/2 realistic case to allow for a systematic $1/N$ expansion. The Hamiltonian is given by^{13,14}

$$\begin{aligned}
 H = & \epsilon_d^0 \sum_i d^\dagger_{i\sigma} d_{i\sigma} + \frac{J}{N} \sum_{(ij)\sigma\sigma'} d^\dagger_{i\sigma} d_{i\sigma'} d^\dagger_{j\sigma'} d_{j\sigma} \\
 & + [\lambda_i [b^\dagger_i b_i + \sum_{\sigma} d^\dagger_{i\sigma} d_{i\sigma} - 1] + \epsilon_p \sum_{i\sigma} p^\dagger_{i\sigma} p_{i\sigma} \\
 & - \frac{2t}{\sqrt{N}} \sum_{\sigma} \gamma_k (d^\dagger_{k+q\sigma} b^\dagger_q p_{k\sigma} + p^\dagger_{k\sigma} d_{k+q\sigma} b^\dagger_q) \quad (9)
 \end{aligned}$$

ϵ_d^0 and ϵ_p are the bare d and p levels γ_k is a hybridization matrix element between the copper and the oxygen while J is a direct copper-copper super-exchange which is generated by integrating our high energy degrees of freedom to generate an effective low energy Hamiltonian. b is again a slave

boson introduced to take care of the single occupancy constraint on the copper site. In the large N approach we introduce order parameters $b = \langle b_i \rangle$ and $\chi_{ij} = \langle d^\dagger_{i\sigma} d_{j\sigma} \rangle$. The boson b plays again the role of coherence or "fermi liquid order parameter". It measures the quasiparticle residue and its vanishing signals the disappearance of the Fermi liquid phase. The phase with $b=0$ is a non fermi liquid phase in which, in the presence of an intrinsic oxygen bandwidth, the oxygen holes form a fermi liquid decoupled to first order from the copper spins.

The phase diagram of this model in the large N limit is very rich and can be summarized in Fig.(2). We will assume that $J \ll t$. Along the $\delta = 0$ axis there is a Brinkman Rice transition when the charge transfer energy $U \equiv \epsilon_p - \epsilon_d^0$ becomes comparable to the hopping t . The order parameter b jumps discontinuously to zero and at the same time the order parameter χ_{ij} jumps from a uniform state for small U to a dimerized state for large U .

Below the Brinkman Rice point the chemical potential μ is continuous while the effective mass m^* is finite at $\delta = 0$. Above the Brinkman Rice point the chemical potential jumps discontinuously at $\delta = 0$.

There is a first order line separating a Fermi liquid regime where χ_{ij} is uniform and $b \neq 0$ to a non fermi liquid phase where the χ_{ij} are dimerized.

The transition occurs when the renormalized fermi energy is of the order of the exchange energy so the location of the first order line separating the Fermi Liquid phase ($\chi_{ij} = \chi$ uniform independent of ij) from the dimerized phase is given approximately by $J = \delta t^2 / (\epsilon_p - \epsilon_d^0)$.

The dimerized phase behaves very differently upon doping depending on the ratio of the spin exchange J to the Kondo exchange $t^2 / (\epsilon_p - \epsilon_d^0)$. When $J > t^2 / (\epsilon_p - \epsilon_d^0)$, $b = 0$ even at $\delta \neq 0$ and the holes go on the oxygen sites, while the magnetic background remains inert. When $J < t^2 / (\epsilon_p - \epsilon_d^0)$ but δ is small the

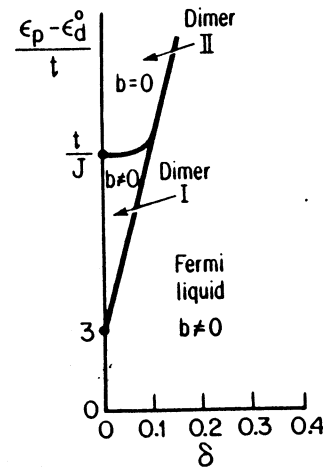


Fig. 2 Schematic phase diagram of Hamiltonian (9) in the $N = \infty$ limit, and for small but finite J . $U \equiv \epsilon_p - \epsilon_d^0$

dimerized copper band mix strongly with the oxygen and the carriers are mixtures of the upper dimer band and the oxygen band. These two regimes (dimer I and dimer II) in the phase diagram of Fig.(2) are separated by a line of first order transitions.

Approaching the uniform to dimer transition from the metallic side one has a strongly correlated fermi liquid with antiferromagnetic spin correlations. Close to this transition the linear coefficient of specific heat γ and the susceptibility χ behave as

$$\gamma \sim \chi = \frac{1}{J + \frac{\delta t^2}{\epsilon_p - \epsilon_d^0}} \quad (10)$$

In the large N approach superconductivity arises from fluctuations around mean field theory. The pairing originates from a screened superexchange interaction between the quasiparticles. The maximum superconducting temperatures indeed occur on the Fermi Liquid side but close to the metal insulator when $\delta t^2/(\epsilon_p - \epsilon_d^0) \sim J$. The superconductivity is in the d wave $\cos k_x - \cos k_y$ channel in agreement with the previous mean field one band results.⁸

The main difference between the copper oxide problem and the heavy fermion problem lies in the different parameter range of the Kondo lattice Hamiltonians. In the heavy fermion problem the oxygen bandwidth is the largest scale in the problem, and it is well in the Kondo regime. The copper oxide systems the oxygen bandwidth is very small compared with the Kondo exchange and the fact that the direct copper copper superexchange is large indicates that one is closer to the mixed valence regime. The treatment of Refs.(13-14) correspond to the strong coupling limit of the Kondo lattice problem in which the resonant impurity level band is pulled out of the continuum of the conduction band as the conduction electron bandwidth is reduced. In the heavy fermion system $T_c(b)$, the Kondo temperature or the fermi liquid coherence temperature, is much larger than the pairing energies which drive it superconducting at low temperatures. This inequality is probably reversed in the high temperature superconductors. The superconductivity would then occur at $T_c(b)$ without ever passing thru a fermi liquid regime. This conjecture is appealing in the light of recent NMR experiments which show that above T_c the temperature dependence of the nuclear spin relaxation rate on the copper and oxygen sites is completely different suggesting that above T_c one is in a phase where $b = 0$ and copper and oxygen are to leading order decoupled while below T_c the spin relaxation rate drops on both sites indicating that the superconductivity affects both oxygen holes and copper spins. Therefore below T_c coherence between copper spins and oxygen holes is established. The existence of very large mass renormalizations in the fermi liquid phase of the heavy fermions and its absence in the copper oxides can be accounted by the fact that the copper resonant level is pulled from the continuum and the fact that close to half filling the renormalized fermi energy is of the order of the exchange energy. As shown by Eq.(10), in this limit the fermi liquid parameters do not depend very strongly on filling factor.

In Refs.(12-13) a zero oxygen bandwidth was assumed. When the oxygen bandwidth becomes comparable with the hybridization energy $t^2/(\epsilon_p - \epsilon_d^0)$ a crossover between the behavior found in Refs.(12-13) and heavy fermion behavior is expected to occur as the doping is increased away from half filling.

References

1. J.G. Bednorz and K.A. Muller, Z. Phys. B64, 188 (1986).
2. P. Coleman, Phys. Rev. B29, 3035 (1984); S. Barnes, J. Phys. F6, 1375 (1976).
3. A. Millis and P.A. Lee, Phys. Rev. B35, 3394 (1987); A. Auerbach and K. Levin, Phys. Rev. Lett. 57, 877 (1986).
4. P.W. Anderson, Science 235, 1196 (1987).
5. C. Varma and Y. Yafet, Phys. Rev. B13, 2950 (1976); T.M. Rice and K. Ueda, Phys. Rev. Lett. 55, 995 (1985).
6. J. Reger and P. Young, Phys. Rev. B18, 5978 (1988).
7. D. Vaknin, S.K. Sinha, D. Moncton, D. Johnston, J. Newsam, C. Safinya, and J. King, Jr., Phys. Rev. Lett. 58, 2802 (1987).
8. G. Kotliar and J. Liu, Phys. Rev. B38, 5142 (1988).
9. G. Baskaran, Z. Zou, and P.W. Anderson, Sol. Stat. Commun. 63, 973 (1987).
10. G. Kotliar, Phys. Rev. B37, 3664 (1988).
11. I. Affleck and Marston, Phys. Rev. B37, 3774 (1988).
12. G. Baskaran and P.W. Anderson, Phys. Rev. B37, 580 (1988); I. Affleck, Z. Zou, T. Hsu, and P.W. Anderson, Phys. Rev. B38, 745 (1988).
13. G. Kotliar, P. Lee, and N. Read, Physics BC, 153-542, 538 (1988).
14. G. Kotliar, Proceedings of the Adriatico Research Conference "Towards the Theoretical Understanding of High T_c Superconductors", to appear in Int. J. Mod. Phys.; G. Kotliar and C. Castellani, to be published in Phys. Rev. B, Rapid Communications.