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Amalfi, Italy 14 – 16 October 1993

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PREFACE

This book arises from the wish to express our gratitude and to pay homage to Maria Marinaro, Dean of the Science Faculty of Salerno University, as a scientist, as a teacher and as a friend, on occasion of her sixtieth birthday; it contains the invited lectures presented at the International Conference "Superconductivity and Strongly Correlated Electron Systems" held in Amalfi, Italy, from 14 to 16 October 1993 and some invited articles on the same field by scientist who have collaborated with her.

When we decided to honour Maria Marinaro, we had to choose between the many topics to which she gave important contributions during her scientific career: Quantum Field Theory, Renormalization, Phase Transitions, Condensed Matter Physics, Superconductivity, Neural Nets, Self-organizing Hierarchical Systems. The choice fell on "Superconductivity and Strongly Correlated Electron Systems", both for the relevance and the great interest of this fascinating and fast-developing research area, and for the presence in the Department of Theoretical Physics of the Salerno University of a research group, directed by her, active in this field.

The volume includes articles on various topics in the field of strongly correlated electron systems and high-T_c superconductivity, such as Hubbard and t–J models, polaronic models for superconductivity, Fermi and non Fermi liquid theories, heavy fermion systems. The authors are specialists in their respective fields and are actively engaged in the study of the problems touched upon by them. For this reason we are confident that this book will attract the attention of the readers and will prove to be useful for researchers involved in Condensed Matter Physics. The ordering of papers is largely arbitrary due to the overlapping among the problems addressed.

Very deep is our gratitude to our colleagues of the Salerno University A.M. Cucolo, M. Fusco Girard, F. Mancini and S. Pace who joined us in the Organizing Committee. To our great regret, Prof Eduardo R. Caianiello passed away few days after the closing of the Conference; grieved and grateful, we want to remember his strong support and contribution to the preparation of this Conference.

We gratefully acknowledge the financial support we received from the Salerno University, the Istituto Italiano per gli Studi Filosofici, the International Institute for Advanced Scientific Studies and from the Assessorato alla Cultura of the Regione Campania.

We express our deep gratitude towards the eminent scientists who have promptly and friendly accepted to give their lectures, and to all the participants who, with their presence and interesting discussions, helped to create a warm and stimulating atmosphere, whose memory will last; a non minor benefit was the wonderful and warm venue of Amalfi, with the beauty of its sea and landscapes and the feeling of hospitality by its people.

July 1994

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Towards a theory of copper-oxide metals

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Abstract

I summarize salient features of the theoretical work in the last two years to obtain the Marginal Fermi-liquid response functions in a model of Copper-oxide metals with finite range interactions.

1 Introduction

The peculiarities of the normal state of copper-oxide based metals are well documented. They imply that these metals cannot be discussed in the framework of Landau Fermi-Liquid theory. Finding the correct theoretical framework is essential before the instability to the superconductive state can be discussed. indeed, superconductivity is most likely a corollary to the anomalies in the normal state.

In our pursuit of the fundamental theory of these metals, we have been guided by two sets of considerations. The first is simply the question, why do these phenomena occur in copper-oxide metals, and not in other transition metal oxides, or sulfides, or selenides, etc.; either quasi-two dimensional or three-dimensional. This led us to suggest a model [1] for the copper-oxides, which is discussed below. The second set of considerations is phenomenological. The normal state anomalies could be understood from an assumption about a scale-invariant change and spin-fluctuation spectrum [2]. Some preedictions made on the basis of this spectrum were soon experimentally verified. Our approach then is to try to derive this marginal

Fermi-liquid spectrum from the proposed microscopic model. Progress in this approach is reviewed here.

2 Microscopic models

As one moves from the left to the right in the periodic table, the second ionization energies of the 3d-transition metals fall by about 8 eV, and for copper is very close to the relevant affinity levels of oxygen. Band structure calculations, which must get the electrostatic energies nearly right, give in a tight binding fit that the Cu level energy $\epsilon_d \approx \epsilon_F$, the oxygen level energy at the self-consistent charge distribution. In such a situation the interatomic electron-electron repulsion, which is responsible for the stability of all transitions metal oxides to begin with, has also an important dynamic role to play. This is the central theme in one of the proposed models for the copper-oxides [1]. The model Hamiltonians, hypothesized as the minimum necessary is

$$H = \epsilon \sum_i (d_{i\sigma}^+ d_{i\sigma} - x_{i\sigma} x_{i\sigma} - y_{i\sigma}^+ y_{i\sigma}) + \sum_{<ij>} (t_{ij} d_{i\sigma} x_{j\sigma} + h.c. + x \to y)$$

$$+ U \sum_i n_{di\uparrow} n_{di\downarrow} + V \sum_{<ij>} \delta n_{di} (\delta n_{xj} + \delta n_{yj}) \qquad (1)$$

Here $\epsilon = \frac{1}{2}(\epsilon_d - \epsilon_p)$ and $< ij >$ denote nearest-neighbor summation.

This model reduces to the Hubbard model, if $E_x \gg U$, where

$$E_x = E(Cu^{2+} + O^{2-}) - E(Cu^+) - E(O^-)\,, \qquad (2)$$

includes renormalization due to V. For $E_x \gg U$, the charge fluctuations δn_x, δn_y on the oxygen atoms are negligible and the last term in (1) has no role. But for $E_x \ll U$, as in Cu-O metals, this term was expected to lead to qualitatively new physics. For $V \sim |\epsilon_d - \epsilon_F| \sim t$, the model cannot be reduced to the Hubbard model for the metallic state. Some conclusion has arisen at this point because at 1/2 filling, in the insulating state, in which there are no low-energy charge fluctuations, the model can be reduced to the Hubbard model.

Several approximate [3] calculations (and one exact calculation [4] on a small Cu-O ring) on this model, suggest that the ground state is superconductive due to charge transfer resonance for $V \geq (\epsilon_d - \epsilon_F) \sim t$. But here our main concern is with the normal state. The model (1) is not solvable exactly. Below, we shall summarize the solution of a model abstracted from (1), which can be solved exactly, and which shows that the copper-oxygen repulsion does indeed lead to qualitatively new non-Fermi-liquid behavior.

3 Phenomenology

In an attempt to find the unifying features in the diverse observed anomalies in the normal state of Cu-O metals, and to constrain the theoretical approaches, a phenomenological form for the spectral function for spin and charge fluctuations was proposed [2]. This marginal-Fermi-liquid spectrum has the following form for $\omega \ll \nu_F q$:

$$\mathrm{Im}\,\chi_{\rho,\sigma}(q,\omega) \sim \begin{cases} N(0)\,\omega/T, & \omega \ll T \\ -N(0), & T \ll \omega \ll \omega_c \end{cases} \tag{3}$$

where ω_c is a cut-off energy. As a consequence, the quasi-particle residue vanishes logarithmically, $Z^{-1} \sim 1 + \lambda\ \ln(\omega, /x)$ where $x = \max(|\omega|, T)$.

The MFL spectrum is intermediate between the analytic itinerant or Fermi-liquid behavior, $\mathrm{Im}\ \chi_{\rho,\sigma}(q,\omega) \sim N(0)\omega/(v_F q)$ and the more singular Curie-type behavior, $\mathrm{Im}\ \chi_{\rho,\sigma}(q,\omega) \sim \omega/T^2$, for localized excitations. In fact a simple "bubble calculation" of the susceptibility using a one-particle propagator which is itinerant $\sim (\omega - \epsilon_k + i\delta\ \mathrm{sgn}\,\omega)^{-1}$ and the other which is localized or momentum independent $\sim (\omega + i\delta\ \mathrm{sgn}\,\omega)^{-1}$ produces the MFL susceptibilities. The crucial thing to understand is how the quantum degrees of freedom get quenched dynamically so that a localized propagator results. Equally important is to localized propagator alone, which would give a too singular, Curie-type, contribution.

The MFL spectrum is a scale invariant spectrum, as in the fluctuation regime of a quantum critical point. The fore-mentioned ω^{-1} propagators should occur as low-energy resonance near the critical point. Superconductivity or localization due to disorder are supposed to serve to cut-off the

large density of low energy excitation in (3). Indeed, a MFL spectrum can be shown (in approximate calculations) to be unstable to superconductivity.

An important point about he MFL spectrum is that the singularities are in the frequency dependence; the momentum dependence is assumed smooth. The singularities have, in other words, a spatially local origin, quite unlike the singularities of the one-dimensional probe.

Predictions of one-particle spectra based on (3), both in the normal and superconductive state, have been verified encouraging one to seek the microscopic basis of the MFL spectra.

4 Summary of solutions to the impurity model

An impurity model abstracted from the model of Eq. (1) was solved recently by Wilson's numerical renormalization group [5]. The spectrum at the mixed-valence point of impurity (such as occurs in the copper-oxide metals, where Cu fluctuates between $Cu^{+}(S = 0)$ and $Cu^{++}(S = 1/2)$ is indeed of the MFL form. We have recently succeeded in solving this model analytically gaining new insights [6].

The impurity model bears the same relationship to this copper-oxide model as Anderson (or Wolff) model for a local moment bears to the Hubbard model. We consider

$$H = \sum_{k,\sigma l} \epsilon_{kl} c^{+}_{k\sigma l} c_{k\sigma l} + \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + t \sum_{k,\sigma} (d^{+}_{\sigma} c_{k\sigma 0} + h.c.)$$

$$+ \sum_{kk'l} V_{kk'l} \left(n_d - \frac{1}{2} \right) \left(\sum_{\sigma} c^{+}_{k\sigma\ell} c_{k'\sigma\ell} - 1 \right) \qquad (4)$$

d is the local orbital, which as required by symmetry, hybridizes only with one point-group channel ($l = 0$). This will be referred to as the hybridizing channel. Other channels, the screening channels, have only the ionic interaction V_l. Given finite t, it does not matter whether or not one keeps V_0 finite. We take $V_0 = 0$.

It is convenient to change the representation to real space operators, specifically to those operating on radial shell-orbitals, defined by Wilson

[7], by logarithmically discretizing momentum (and frequency) by a scale factor λ. The n-th shell-orbital peaks at a distance $k_F^{-1}\lambda^n$ from the impurity. The Hamiltonian in such a representation is $H = H_0 + H_{KIN}$ where the local and kinetic energy part read

$$H_0 = \frac{\lambda^{1/2}}{1+\lambda}\left[\epsilon_d\left(n_d - \frac{1}{2}\right) + U n_{d\uparrow} n_{d\downarrow} + t\sum_\sigma d_\sigma^+ h_{0\sigma}\right]$$
$$\left[+\sum_{l,\sigma} V_l\left(n_d - \frac{1}{2}\right)\left(s_{0l\sigma}^+ s_{0l\sigma} - \frac{1}{2}\right)\right]$$
$$H_{KIN} = \frac{1+\lambda}{2\lambda}\sum_{n,\sigma}\lambda^{-n/2}(t_n h_{n\sigma}^+ h_{(n+1)\sigma} + t_n s_{n\sigma}^+ s_{(n+1)\sigma} + h.c.) \qquad (5)$$

Here h denotes the hybridizing and s the screening channels. It can be shown that the screening channels $l = 1...N$ can be replaced by a single spinless screening channel with a coupling constant $\bar{V} = \sqrt{N}V$, with all $V_\ell = V$. The screening interactions are then simply

$$\bar{V}\left(n_d - \frac{1}{2}\right)\left(s_\sigma^+ s_\sigma - \frac{1}{2}\right) . \qquad (6)$$

The physical idea in the proposed route [8] to the breakdown of the Fermi-liquid and quasi-particle concepts followed here, is that for ionic interactions $\bar{V}$ above a critical value, local multi-particle resonance form at the chemical potential, drawing weight of the one-particle or hole spectra from higher energies on he scale of the charge transfer gap in the insulating state. This one-particle-hole weight is largely incoherent. The multi-particle resonance can not be constructed perturbatively, putting in jeopardy the Landau scattering between the low-lying excitations of the interacting and noninteracting fermions. Recall the scattering involving incoherent parts is assumed benign in Landau Fermi-liquid theory, and safely absorbed in the Landau parameters. To form these low energy resonance, we consider $U, \bar{V} \gg t$. Actually, we will take $U \to +\infty$, (only Cu^+ and Cu^{++} allowed). We can now diagonalize the spectrum of the impurity. The two lowest states are

$$\eta^+|0> = |0,1>, \quad \text{with energy} \quad E_\eta = -\frac{\bar{V}}{4}$$
$$\varsigma_\sigma^+|0> = |\sigma,0>, \quad \text{with energy} \quad E_\varsigma = \frac{\epsilon_d}{2} - \frac{\bar{V}}{4} - \sqrt{\left(\frac{\epsilon_d}{2} - \frac{\bar{V}}{4}\right)^2 + t^2} \qquad (7)$$

where in the bras. the first number is the charge and spin of the impurity plus the hybridizing channel and second, the charge of the screening channel. Other states are separated by energies of a least V. The states in (7) satisfy the important physical requirement of the Friedel screening sum-rule. Mixed-valence is achieved in (5) for $E_\eta \approx E_\zeta$. In fact is is impossible to obey Friedel sum-rule in the mixed-valence situation for models of the form (4) without terms proportional to V_1.

The next step is to re-express the Hamiltonian in the impurity basis: $\eta^+|0>$ and $\zeta_\sigma^+|0>$. In this basis set, the couplings are all small and bosonization methods can be used. it turns out that the low energy Hamiltonian can be reduced to a quadratic form:

$$H_{low-energy} = t\sum_n \lambda^{-n/2} s_n^+ s_{n+1} + \hat{t} s_o^+ \alpha^+ + h.c.\,, \tag{8}$$

about which the corrections can be calculated perturbatively. Here $\alpha = \frac{1}{\sqrt{2}}(\zeta_\sigma + \zeta_{-\sigma})$. The noteworthy feature of (8) is that only one combination, α, of the local spin operators is hybridized with the conduction electrons; the other $\beta = \frac{1}{\sqrt{2}}(\zeta_\sigma - \zeta_{-\sigma})$ is free. The propagator $<\beta^+(\omega)\beta(0)>$ is then free $\sim 1/(\omega + i0^+)$, while $<\alpha^+(\omega)\alpha(0)>$ have a scale γ: $<\alpha^+(\omega)\alpha(0)> \sim (\omega + i\gamma)^{-1}$, where $\gamma \approx \pi\hat{t}^2/t$. Physical properties involve convolutions of the two and the resulting spectrum is precisely of the marginal Fermi-liquid form.

5 The problem of the lattice

It turns out that, the methods outlined above can be used to solve the two impurity problem, as well [6]. We find that at mixed-valence the isolated impurity critical point is stable to inter-impurity interactions. This comes about because we have only relied on the condition for mixed-valence $< n_d >= 1/2$ to obtain the critical point. No special symmetries of the single impurity problem, lost in the two impurity problem or the lattice, are used.

The one-particle Green's function for the impurity problem has also been determined. The leading self-energy of the itinerant electrons in of the form $\omega\ ln\ \omega + i\omega \mathrm{sgn}\,\omega$. But there is also a localized (momentum independent) contribution whose spectral weight is $\sim (\theta(\omega)/ln|\omega|)\mathrm{sgn}\,\omega$. It

is very tempting to suggest that the large momentum independent background found experimentally by angle resolved photoemission is this component. This result also does not change in the two impurity problem. We also find that the pairing susceptibility of conduction electrons both in the single and two-impurity problems also diverges.

One of the themes running through this work is that fluctuations both in charge and spin becomes localized due to dynamics, with the one-particle spectra retaining itinerant character. We hope to use this to understand the observed difference in the nuclear relaxation rate on Cu and on oxygen using specifically the fact that the ω^{-1} divergence occurs only at the site of large U, i.e. on Cu.

In the one or two impurity problem, one has to tune parameters to be at the mixed-valence critical point. Othrwise for $E_\varsigma >$ or $< E_\eta$ the fixed-point is that of a Fermi-liquid. The cross-over temperature from MFL to FL has been discussed in Ref. [10].

We have also succeeded in finding a mean-field solution of the single impurity problem which reproduced the exact results. We envisage solving the lattice problem by using such a solution, by embedding an impurity in a self-consistent medium. Two new issues arise in the lattice problem. First, the impurity [11] interaction with the medium involves only one-particle Green's functions of the latter. These (in a self-consistent solution) have only logarithmic corrections over the free one-particle Green's function used in the solution of the impurity problem above. One must ensure that these logarithmic corrections do not invalidate the solution. Secondly, the domain of attraction of the critical point is quite different than in the impurity problem. For a fixed set of parameters, one must determine the chemical potential as a function of total charge near the mixed-valence point. This is much like determining the co-existence curve in the gas-liquid transition problem. We expect that over a range of electron-densities, the mixed-valence critical point is rendered attractive or the cross-over to Fermi-liquid is very slow. Some calculations in this regard are presented in Ref. [5].

A more general solution [9] to the lattice problem not using mean-field theory is also being pursued. The important trick is to express the screening conditions near the valence degeneracy in terms of a gauge-field and to show that a systematic low energy theory can be constructed.