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ABSTRACT

This paper describes certain aspects of Highly Correlated Systems (HCS) such as high Tc superconductors (HTSC) and some new class of Heavy Fermion (HF) systems which have been studied recently. The problem is discussed on how the charge and spin degrees of freedom participate in the specific character of superconductivity in the copper oxides and competition of the magnetism and Kondo screening in heavy fermions. The electronic structure and possible superconducting mechanisms of HTSC compounds are discussed. The similarity and dissimilarity with HF compounds is pointed out. It is shown that the spins and carriers in the copper oxides are coupled in a very nontrivial way in order to introduce the discussion and the comparison of the Emery model, the $t-J$–model and the Kondo–Heisenberg model. It concerns attempts to derive from fundamental multi–band Hamiltonian the reduced effective Hamiltonians to extract and separate the relevant low–energy physics. A short review of the arguments which seem to support the spin–polaron pairing mechanism in HTSC are presented. Many other topics like the idea of mixed valence states in oxides, the role of charge transfer (CT) excitations, phase separation, self–consistent nonperturbative technique, etc. are also discussed.

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1 Introduction

A satisfactory overall picture of the HCS is still in the process of evolution. Correlation effects(CE) are of great importance in determining the properties of many substances, especially for description of the magnetism in transition metals and their compounds, metal-insulator transition, heavy fermions, etc.[1]. Recently, with the discovery of HTSC, many theoretical investigations on its mechanism have been done invoking the strongly correlated models [2]–[4]. The understanding of the true nature of the electronic states in HTSC and HF are one of the central topics of the current experimental and theoretical efforts in the fields [5]. The plenty of experimental and theoretical results show that the charge and spin fluctuations induced in the carrier hopping lead to the drastic renormalization of the single-particle electronic states due to the strong electron-correlation. It makes the problem of constructing of the correct wave functions of carriers and description the real many-body dynamics of the relevant correlation models of HTSC and HF quite difficult. Unfortunately, we have, at the present time, no generally accepted and complete formal theories the HTSC and HF. But we do have a number of relatively well developed approaches to the theory, which describe some selected set of experimental results and are connected with single favorite picture for the mechanism of HTSC or formation HF state.

It is formidable task to get a complete picture of what has been done thus far in these quickly growing areas of research. The main purpose of the present discussion is to indicate some new trends and perspectives in this fascinating field. Recent investigations on HTSC [6]–[13] and HF [14]–[28] have brought forth significant reconsideration in our understanding of these controversial and still unsolved problems. The purpose of this paper is to discuss a class of relevant correlation models in which arise questions of fundamental condensed matter theory interest. Our focus will be on the self-consistent description of the HCS under consideration. It seems appropriate to point out that a number perturbation-theory or mean-field theory approaches to the strongly correlated models which have been proposed by many authors in the past few years, are in fact questionable or inadequate [29]–[31].

To clarify this point, let me first sketch the general situation, before I attempt to give a more detailed survey. As was mentioned before, the most characteristic feature of the recent advancement in basic research on electronic properties of solids is development of variety of the new class of materials with unusual properties: high Tc superconductors, heavy fermion compounds, magnetic and diluted magnetic semiconductors, magnetic superlattices etc. Contrary to the simple metals, where the fundamentals very well known and the electrons can be represented in a way such that they weakly interact with each other, in these materials the electrons interact strongly and moreover their spectra are complicated, i.e. have many branches etc. This give rise to interesting phenomena such as magnetism, metal-insulator transition, heavy fermions etc, but the understanding of what is going on is in many cases only partial if exist at all. Therefore the theoretical studies of the Highly Correlated Electronic Systems(HCES) are very important and actual. A principle importance of these studies is concerned with a fundamental problem of electronic solid state theory, namely with the tendency of 3d electrons in transition metals and 4f electrons in rare-earth metal compounds and alloys to exhibit both localized and delocalized behaviour. The interesting electronic and magnetic properties of these substances are intimately related to this dual behaviour of electrons. In spite of experimental and

theoretical achievements, still it remains much to be understood concerning such systems. A satisfactory overall picture is still in the process of evolution. The extensive study of high Tc oxides is, of course, most important, but we should not forget the fact that there remain some other basic problems unsettled. For instance, another problem of strong correlation in heavy fermion systems still unsolved.

In order to match such a trend we need to develop a systematic theory of the Highly Correlated Systems, to describe from the first principles the condensed matter theory and statistical mechanics the magnetic and superconducting properties of this class of materials. In this paper we shall discuss briefly the approach to the HCES which has been initiated by us in Dubna two decades ago. A number of other approaches for HCES have been proposed. The approach we have proposed in an extensive list of papers are believed is very suitable for description of the strongly correlated many-body systems with complicated spectra. It is quite revealing during the consideration of HCES to follow the logic of development of many-body techniques. This logic is well known. The simple Hartree-Fock or RPA treatment of the correlation between electrons omits several essential features. One of them is the damping of quasiparticles. Usually, this latter problem requires much larger theoretical efforts. However, this must be final goal towards a real understanding of the many-body dynamics in HCES. Our method allows one to describe completely the quasiparticle spectra with damping in a very natural way. This approach has been suggested as essential for various many-body systems and we believe that it bear the real physics of Highly Correlated Systems.

2 The Electronic Structure of HTSC

Before starting a discussion on the physics of HTSC, it is very important to know their electronic structure and furthermore the nature of the states induced on the Fermi level by a chemical substitution or stoichiometry changes. To obtain information of the above type one must carry out realistic band-structure calculations. Such calculations, which have been performed in numerous paper [32],[33], give a very detailed description of the one-particle electronic states in these materials [34]–[44]. It is well known that transition metal oxides are classified [39] into two categories: CT materials and the Mott-Hubbard ones. High temperature superconducting oxides belongs to the first class of materials [40]–[43]. This is because of the subtle balance of the energy levels in copper and oxygen ions and of the unique crystal structure. In CT phase the Cu-O-planes behave as rather highly ionic system; a rapid metallization occur upon doping. It is worthy to emphasize that there are the crucial difference in the electronic properties between CT and MH materials [32]–[43].

The calculated electronic structure has been checked by comparison to experiments such as photoemission, optical reflectivity, Raman scattering and recently to soft X-ray absorption measurements [44], which has allowed to analyze in a detail of the low energy electronic states [45],[46].

However,the one-particle band theory show up a well known problem, which is related to the breakdown of the one-particle electron-band description due to the strong Coulomb interaction among the electrons in the Cu-O planar complex. The nature of quasiparticles cannot directly be derived from density functional calculations. Nevertheless, the band

structure calculations give an idea how to select the relevant electronic degrees of freedom and to calculate the effective screening of various bare parameters of the suitable effective model Hamiltonians [47]–[49]. We can conclude that the HTSC compounds are strongly correlated systems showing various types of insulating and metallic states induced by the chemical substitution or stoichiometry changes. This gives the heuristics for the searching of an appropriate model Hamiltonians.

In order to give a more complete picture of the electronic states in oxide materials let us discuss shortly an additional intriguing question, namely valence concept of Cu in oxides [50]. As have been formulated in Ref.[51], since the discovery of the HTSC one of the central question is the formal valence of copper in these systems [52], [53]. The situation with this question is rather unclear. Additional complexities come from the controversy of various experimental results. The chemical theoretical arguments supporting the idea that some of the Cu atoms must have a valence of 3+ instead of the more common 2+ has been presented in papers [51]–[56]. These former proposals have led to the following conjectures. In materials such as the copper oxides and related superconducting ceramics there are strong covalent interactions(see also [6]) between oxygen and metal in addition to ionic binding. The resulting charge sharing costs douht on the use of formal ionic charge assignments for reliable models of the electronic states. These considerations are of considerable importance in the attempts to discover superconducting pair-formation mechanisms, especially those which suppose disproportionation reaction such as $(2(Cu^{2+}) \Longrightarrow (Cu^{1+}) + (Cu^{3+}))$ and magnetic coupling among the $d(n \pm 1)$ electrons [55],[56].

There are a number of papers where charge distribution and valence in copper oxide crystals related to superconductivity have been investigated [50]–[61]. For example, in paper [55] a model for interpretation of X-ray-absorption near-edge structure(XANES) have been proposed. The arguments of the evidence of simultaneous Cu^{2+} and Cu^{3+} valences have been presented. Contrary to this statement, in paper [62] on the basis core-level spectroscopic measurements of several cuprate perovskites the claim has been made that trivalent Cu is clearly excluded. Moreover, the failure to superconduct in the rare-earths Ce- and Pr-based perovskites they connect with the fact that the valence of Ce and Pr is more than 3+ in these materials [63]. On the other hand, analysis of the core-level photoemission spectra of the superconducting cuprates, given in paper [64] lead to evidence for a strongly mixed-valent state(see also [65]). The most balanced point of view on this problem has been presented recently in paper [66].

In spite of that fact that we lack a rigorous and definitive foundation of the problem, there are a number of interesting attempts to propose correlated-valence-fluctuation-models for HTSC [67]–[70]. We have therefore concluded, from all of these considerations, that at this stage, most theoretical pictures concerning the valence concept in cuprates are still quite raw and their fate depends ultimately on experimental findings.

3 THE MODEL HAMILTONIAN

The study of the electronic structure in the oxides show that the strong electron correlation forces electrons to localize in the atomic orbitals. On the other hand, the kinetic energy is reduced when electrons are itinerant. Therefore, both these effects should be taking into

account simultaneously. As far as the CuO-planes in the HTSC compounds are concerned the natural model for electronic structure with which one can start to discuss the electronic properties of HTSC is the following multi-band Hubbard model [1]–[5],[33],[48]:

$$
\begin{aligned}
H &= \sum_{i\sigma} \epsilon_d d^+_{i\sigma} d_{i\sigma} + \sum_{lm\sigma} \epsilon_p p^+_{lm\sigma} p_{lm\sigma} + \sum_{\langle i;lm\rangle} (t_{pd\sigma} p^+_{lm\sigma} d_{i\sigma} + h.c.) + \qquad (1)\\
&+ \sum_{\langle lm;l'm'\rangle} (t_{pp\sigma} p^+_{lm\sigma} p_{lm\sigma} + h.c.) + \sum_i U_d n_{i\uparrow} n_{i\downarrow} +\\
&+ \sum_{\langle i;lm\sigma\sigma'\rangle} U_{pd} n_{lm\sigma} n_{i\sigma'} + \sum_{l,m\sigma\neq m'\sigma'} U_{pp} n_{lm\sigma} n_{lm'\sigma'} +\\
&+ \sum (K_{pd} p^+_{lm\sigma} p_{lm\sigma'} d^+_{i\sigma'} d_{i\sigma} + K_{pp'} p^+_{lm\sigma} p_{lm\sigma'} p^+_{l'm'\sigma'} p_{l'm'\sigma}).
\end{aligned}
$$

This Hamiltonian include the various intraatomic (U_d, U_{pp}) and interatomic ($U_{pd}, K_{pd}, K_{pp'}$) Coulomb integrals in each unit cell and is written in hole notation relative to a filled shell ($3d^{10}, 2p^6$) configuration. The only $3d_{x^2-y^2}$ orbitals on the Cu-sites and $2p_{x,y}$ orbitals on the O-sites are considered. It is worthy to mention, that this approach has been proposed by Emery [71]. Starting from an extended Hubbard model he has shown that, for a reasonable range of model parameters, each copper site should have a single hole for a half-filled band. Because of the Hubbard's gap at the Fermi energy, doping lead to holes in the O 2p-band with no change in occupation of the Cu 3d-states. In this picture, the possible superconductivity can results from pairing of the O 2p-holes via relevant exchange interactions.

The above Hamiltonian consist of those terms which are of importance in influencing the physical properties of the studied systems. The type of question which becomes particularly interesting now is the values of the parameters of Hamiltonian (1). It is clear that depending on the values of these parameters, different limiting behaviours can occurs. It follows from Ref.[33]-[49] that the values of relevant parameters for La_2CuO_4 are:

$$
\begin{aligned}
&\Delta = \epsilon_p - \epsilon_d = 3.6 \text{ eV}; \quad t_{pd} = 1.3 \text{ eV}; \quad t_{pp} = 0.15 \text{ eV}; \quad U_d = 10 \text{ eV};\\
&U_p = 4 \text{ eV}; \quad U_{pd} = 1.2 \text{ eV}; \quad U_{pp} = 0; \quad K_{pd} = -0.18 \text{ eV and } K_{pd} = -0.04.
\end{aligned}
$$

According to the classification scheme of Ref.[39] this compound is a CT insulator. For the doped material, the extra hole goes into an oxygen orbital and form a singlet state, as has been proposed by Zhang and Rice [72]. The original approach of Zhang and Rice has led to considerable discussion in the literature [40]–[49], [71]–[77]. In fact the essence of this discussion connected with the most important question on validity and limitations of the reduction from multi-band to one-band model. Zhang and Rice, using the perturbation theory with the small parameter

$$\frac{t_{pd\sigma}}{\Delta} = 1/3,$$

have shown the possibility to reduce of complicated model (1) to the one-band model. They estimated the Heisenberg n.n.exchange coupling in the framework of Anderson's superexchange theory. The result is [48]:

$$J = \frac{4t^4_{pd\sigma}}{\Delta^2 U} + \frac{4t^4_{pd\sigma}}{\Delta^3}.$$

As regards to the effect of doping, Zhang and Rice in details examined the case that $U > \Delta$. In this case, the added holes sit primarily at oxygen sites. Furthermore, they have formulated the new notion, namely *SPIN SINGLET* states of two holes on the square Cu-O complex. Using this original concept, they considered the way how to maximaze the gain from hybridyzation energy, $t_{pd\sigma}$, in second-order perturbation theory. With two holes on Cu-O complex this is achieved by placing the second hole in a combination of the O-p-orbitals with the same symmetry as the central $3d_{x^2-y^2}$. The binding energy (relative to the non-bonding state) of the ZR-Spin-Singlet is:

$$E_{singlet} = -8t^2_{pd\sigma}\left(\frac{1}{\epsilon_p - \epsilon_d} + \frac{1}{U - \epsilon_d - \epsilon_p}\right).$$

The binding energy is relatively strong, so it is possible to suggest that the low energy properties will be governed by these singlet as has been conjectured by Zhang and Rice. The most obvious objection is that the singlet state on one CuO_4 complex has a considerable overlap with that on neighboring squares. In the limit of small hole doping, when the n.n.hopping term $\frac{-1.5t^2}{\Delta}$ is small, the charge will be carried by the tightly bound singlets moving in the S =1/2 background which in turn are coupled by a Heisenberg interaction term. This procedure give a justification of the following $t-J$-Hamiltonian [48]:

$$H = \sum_{ij\sigma} \left(t_{ij}(1 - n_{i-\sigma}) d^+_{i\sigma} d_{j\sigma} (1 - n_{j-\sigma}) + h.c.\right) + J \sum_{ij} S_i S_j. \qquad (2)$$

This Hamiltonian play an important role in the theory of HTSC. Many theoreticians believe that as regards to HTSC it must be visible in framework of $t-J$-model. The recent calculations of spectral function for three-band model on finite clusters and analysis of PES experiments [40]–[49],[75]–[77] seems confirm the existence of peak in observable structure, corresponding in energy and spin with the peak identified with the ZR-singlet. The more refined and detailed measurements will clarify further this intriguing problem. Notice, that the same form of the Hamiltonian(2) follows from one-band Hubbard model after canonical transformation. Indeed, following the pioneering works of Chao,Spalek and Oles [79],[80] and Takahashi [81] who derived the EH of the Hubbard model by a canonical perturbation expansion, it is possible to formulate the $t-J$-model. This procedure has some subtleties as has been explained in the comprehensive discussion recently [72],[74],[81]–[85]. Furthermore, since the two models of interacting fermions, the Hubbard and Anderson models [78], have much in common, the same approach has been applied to the last model. Namely, for Anderson lattice model the EH [86] has been derived with the same method. Cyrot [87] has put forward a similar approach starting from degenerate Hubbard model. In the case of orbital degeneracy, however, the corresponding energy resulting from the virtual transition of the d-electrons to neighboring sites, depends not only on the magnetic structure, but also on the particular orbitals that are occupied at the neighboring sites.

4 The Effective Hamiltonians

The results of the preceding Section show that for the multi-band lattice Hamiltonian(1) it is possible to construct an EH which replaces interconfigurational hopping processes by effective interactions. This is the suitable way to define and describe the low-energy physics correctly. It will be quite revealing to discuss in a more detail how the initial model Hamiltonian can be transformed to new EH in order to clearly bring out the possible superconducting mechanism which is intrinsic of the model. In spite of a number of theoretical studies on this subject, still there are different opinions [71]-[74],[88]-[90] about final form of the relevant transformed Hamiltonian and therefore of the low-energy-scale physics of cuprates. The high energy states of the considered model (1) are doubly occupied states which can be projected out only if we suppose that the low and high energy scales can be decoupled. It is worth mentioning that sometimes the radical opinion is expressed that in the case of HCS the only way to deal with the problem is to construct the effective low-energy Hamiltonian or Lagrangian. It seems that more complex and complimentary approach, accounting more faithfully for the high-energy and low-energy physics may be necessary. However for description of the low-energy physics the construction of the relevant EH should be very useful procedure.

For our purposes it is convenient to discuss the derivation of the EH for multi-band model (1) following to paper [91] where the clever computational procedure has been developed. Let us start from the following Hamiltonian for CuO_2 layer:

$$H = \epsilon_d \sum_{i\sigma} n^d_{i\sigma} + \epsilon_p \sum_{l\sigma} n^p_{l\sigma} + U \sum_i n^d_{i\uparrow} n^d_{i\downarrow} + t \sum_{i\sigma} \sum_{l\neq i} (-1)^{\alpha_{il}} (d^+_{i\sigma} p_{l\sigma} + h.c.) \qquad (3)$$

which is minimal version of the Hamiltonian (1). The phase factor α is:

$$(-1)^{\alpha_{il}} = \pm 1 \text{ if } \mathbf{R_l} = \mathbf{R_i} \mp \mathbf{1/2 e_x};\ \mathbf{R_l} = \mathbf{R_i} \pm \mathbf{e_y}$$

in units of the Cu-O distance. The values of parameters correspond to the strong-coupling regime $t \ll \Delta, (U-\Delta)$. The single occupation of the d-hole states is supposed. EH to the order of t^2 reads

$$H^2_{\text{eff}} = H^2_{\text{kin}} + H^2_{dp} + H^2_{\text{double}} \qquad (4)$$

where

$$H^2_{\text{kin}} = T(-4 \sum_i n^d_i + \sum_{i\sigma} \sum_{lm} (-1)^{\alpha_{il}+\alpha_{im}} p^+_{l\sigma} p_{m\sigma}), \qquad (5)$$

$$H^2_{dp} = I_{dp} \sum_{ilm} (-1)^{\alpha_{il}+\alpha_{im}} (s_{lm} S_i - \frac{1}{4} n^p_{lm} n^d_i), \qquad (6)$$

$$H^2_{\text{double}} = T \sum_{ij\sigma} d^+_{i\sigma} d_{j\sigma} + \frac{1}{4} I_{dp} (8 \sum_{i\sigma} n^d_{i\sigma} n^d_{i-\sigma} - \sum_{ij\sigma} d^+_{i\sigma} d_{j\sigma} (n^d_{i-\sigma} + n^d_{j-\sigma}) + \qquad (7)$$
$$+ \sum_{i\sigma} \sum_{lm} (-1)^{\alpha_{il}+\alpha_{im}} (d^+_{i\sigma} d^+_{i-\sigma} p_{m-\sigma} p_{l\sigma} + h.c.)).$$

Here

$$T = \frac{t^2}{\Delta};\quad I_{dp} = 2t^2 (\frac{1}{\Delta} + \frac{1}{U-\Delta});\quad n^d_i = \sum_\sigma n^d_{i\sigma}.$$

$$\mathbf{S_i} = 1/2 \sum_{\sigma\sigma'} d^+_{i\sigma} \sigma_{\sigma\sigma'} d_{i\sigma'};\quad s_{lm} = 1/2 \sum_{\sigma\sigma'} p^+_{l\sigma} \sigma_{\sigma\sigma'} p_{m\sigma'}.$$

Note that this EH has been derived for large but finite U with the explicit expression for H^2_{double}. The term H_{dp} describes the Kondo-like interaction [78].

The forth order in t EH has been derived in a similar way [91] provided that $Cu2^+$ state should be stable upon doping. The result is:

$$H^4_{\text{eff}} = H^4_{\text{kin}} + H^4_{dp} + H^4_{dd} + H^4_{pp} + H^4_{dp}. \qquad (8)$$

The most interesting terms are given by

$$H^4_{dd} = 2J_{dd} \sum_{ij} (\mathbf{S_i S_j} - \frac{1}{4} n^d_i n^d_j), \qquad (9)$$

$$H^4_{dp} = -2J_{dp} \sum_i \sum_{lm} (-1)^{\alpha_{il}+\alpha_{im}} (s_{lm} \mathbf{S_i} - \frac{1}{4} n^p_{lm} n^d_i) + \qquad (10)$$
$$+ 2\tilde{J}_{dp} \sum_{ij} \sum_{lr} (-1)^{\alpha_{il}+\alpha_{jr}} \left(\mathbf{s_{lr}} (\mathbf{S_i} + \mathbf{S_j}) - \frac{1}{4} n^p_{lr} (n^d_i + n^d_j) \right).$$

Where J_{dd}, J_{dp} and $\tilde{J}_{dp}$ are proportional to $\frac{t^4}{\Delta^3}$. The more details are given in Ref.[91]. To get a complete EH in the limit $U \to \infty$, excluding the double occupied states, the projection procedure has been done

$$H\text{eff} = H(\epsilon_d) + H(\epsilon_p) + H^2_{\text{kin}} + H^2_{dp} + \qquad (11)$$
$$+ H^4_{\text{kin}} + H^4_{dp} + H^4_{dd} + H^4_{pp} + H^4_{dpp}$$

This final EH describes the mobile O holes and strictly localized Cu spins. It is interesting to note that in the limit $U \to \infty$ all the 4-th order contributions to H_{eff} survive. Thus, in addition to the Emery model and single-band $t-J$ model, the present derivation lead to the Kondo-Heisenberg model, which describe the system of fermions coupled to the antiferromagnetic spin system. The presented form of the EH may be compared with a number of variation on this theme by other authors [71]-[99].

5 Coexistence of Spin and Carriers Systems

In the undoped systems there are a uniform charge distribution and strong antiferromagnetic correlations between copper spins. The reduced models reveal essential local physics arising from the strong Cu-O and O-O hybridization overlap. How doping will modify the charge and spin distribution of the system? Contrary to the insulating behaviour the doped systems still are not completely understood and create a number of controversy [40]-[50]. At low doping the charge inhomogeneity in the system is small and antiferromagnetic fluctuations are weaker than in insulator. The formation of localized states within the gap (correlated states) are also clearly observed in most HTSC compounds. Recently a very detailed analysis of the doped systems and the nature of carriers

has been given in papers [9],[100],[101] from a spectroscopic point of view. Charge carriers are introduced when the number of holes increases beyond one per unit cell. It has been argued that there are a number of features point towards a breakdown of the Fermi liquid picture. The structure of the valence band can only be interpreted by including strong correlations. The presence of the Cu d^8 satellite at roughly 13 eV clearly indicates the presence of strong correlation between holes on a copper site. The strong reduction of the bandwidths is another manifestation of HCS. A third point are the characteristic features of the transfer of spectral weight, which is definitively a many-body effect.

Thus, the analysis of the experimental data as well as the calculations on model Hamiltonians of correlated systems (which also lead to strong renormalizations of the bandwidth) show that the carriers are not weakly coupled free particles, but they are complicated objects(see also [102]) such as ZR-singlets or other higher dressed quasiparticles. That confirm the statement that the question about true nature of carriers in the copper oxides are one of the central in the field and are still open.

The study of spin fluctuations in the doped phase remains also a quite open subject and is not well understood . In the framework of $t-t'-J$ model the doped holes are approximated by the ZR singlets moving in the $Cu-O_2$ plane. This motion include the "correlated hopping" processes. As regards to the dynamics of triplet states, it is not crucial for HTSC compounds up to doping for which Tc is at its maximum. The detailed reconsideration of the superexchange in cuprates [101] which include the processes of double occupancy of a copper and oxygen atoms show that the repulsion between nearest neighbor ZR singlets is a very important process. Contrary to the accounting for ZR triplets, Sawatzky et al [101] have proposed the new picture of the non-orthogonal singlets. If their estimations are correct, then the scheme of "phase separation" is not very likely.

The approach which is based on the idea of "phase separation" [8],[103],[104] has attracted much attention recently. It was shown that in framework of $t-J$ model, that in absence of long-range Coulomb interaction, a low concentration of holes is unstable to phase separation into a hole-rich phase and a hole-deficient antiferromagnetic phase. This is seems the result of competition between tendency of the carriers in correlated systems to the formation of antiferromagnetic bonds and mobile-carrier concentrated regions. The main conjecture of this approach is that the most important interaction, which define the low energy properties, is the scattering of mobile holes from the large amplitude collective modes which have been called "local dipolar modes". The analysis which has been made in several recent papers [8] confirm the occurrence of phase separation in correlated models, including $t-J$ and $t-J-V$ one-dimensional models. The variational calculations [103] within Emery model show temperature dependent phase separation region. The parameter dependence of the maximum temperature of phase separation shows the same tendency as the empirical parameter dependence of HTSC transition temperature. An important practical consequence of the above results is that the spins and carriers in the copper oxides are coupled in a very non-trivial way. Within an effective single-band $t-J$ model the magnetic degrees of freedom play a main role as well as for an explanation to the normal-state properties and to the pairing mechanism. The role of the copper and oxygen charge degrees of freedom needs the additional studies. It was suggested sometime ago[105] that the charge degrees of freedom could play an important role when the Coulomb repulsion between nearest neighbor is the same order as t_{dp} and Δ. It is worthy to note that the presence of multi-band structure and a nearest-neighbor repulsion of the

order of the bandwidth are very vital factors [10],[11],[90],[106]–[108]. Recently it was shown in the weak coupling approximation in Ref.[109] that the phase separation always exist near the CT instability region. Quite recently the role of collective modes on the charge transfer instability(CTI), phase separation and the superconductivity has been analyzed in a detail within the extended Hubbard model [10],[11]. The dynamics of the charge degrees of freedom for the CuO_2 planes in copper oxides has been described in the weak- and strong-coupling limit. In both cases the charge degrees of freedom affect the low-energy properties. The CTI promote the phase separation and a pairing instability. The closely related problem is the metal-charge-transfer-insulator(MCTI) transition at the half-filling [90]. It is important to realize that the metal-insulator transition is an essentially strongly correlated effect which can be described in the strong-coupling formalism only. The mean-field analysis of the strong-coupling limit could give the qualitative picture only, which may be seriously modified by using the refined self-consistent method [29],[30],[90].

Since the honest theoretical treatment of the all above mentioned problems is very complicated, perhaps it is instructive to look again at the physics involved. Let us discuss briefly, to give a flavor only, the very intriguing problem of the relevance of the spin-polaron pairing mechanism in the copper oxides. An interesting proposal has been made some time ago by Kamimura [110], who has first pointed out that the inclusion of two bands of $d_{x^2-y^2}$ and d_{3z^2} types, interacting by the Hund's coupling as well as the electron correlation could play an important role for HTSC. It was shown that the interplay of Hund's coupling and superexchange interactions between holes in the $d_{x^2-y^2}$ band give rise to an effective attractive interaction between spin-polarons created in d_{3z^2} by doping. When a certain number of spin-polaron are created, they form spin-singlet pairs. These spin-polaron pairs are boson-like particles constructed from fermions, and the Bose-Einstein condensation occur below a condensation temperature.

This attractive picture seems was not very popular till now mainly because of lack of the direct (or indirect) experimental confirmation. Nevertheless, the idea of a carrier as a higher dressed object gradually obtained a recognition. The ZR singlet is in essence a polaron of a small radii. The "spin-bag" concept which is related deeply to the problem of interplay between antiferromagnetism and superconductivity, is based on certain extension of the pairing theory beyond the Fermi-liquid regime in terms of spin polaron. In the framework of the Emery model the oxygen-site hole will hop from site to site not as a bare carrier, but as a dressed object too, polarizing the surrounding spins. This situation resembles the case of the magnetic semiconductors [111]–[113], where under various regimes the bare carriers can be greatly renormalized and the relevant true carriers must be considered;however the physics involved is somewhat different. Investigation of the magnetic polaron [111] permit us to clarify the nature of the true carriers at low temperatures. An interesting analysis of the questions of valency, correlation, magnetism and the nature of the charge carriers in cuprates has been given in Ref.[115]. The result of this analysis was claiming that the carriers are neither weakly coupled free particles nor spin polarons, but are something new: "spin hybrids", consisting of a coherent and nonperturbative mixture of local spin-orbital electronic configurations, some of which represent deviations in the local antiferromagnetic order. More advanced approach has been proposed in a series of papers [116]–[119]. The detailed investigation of the problem of the magnetic polaron within $t-J$ model has been performed in Ref.[120]. The list of various attempts for construction of a suitable magnetopolaronic states for cuprates is extensive [115]–[135].

Unfortunately, the main question whether the experiment confirm any given picture of the spin polaron pairing mechanism is not clear [133]–[135]. The more detailed review of the experimental results and the interesting qualitative suggestions have been done by Mott [134],[135] recently.

6 Competition of Interactions in Kondo-Systems

Intersite correlation effects in metal alloys and, especially, in anomalous rare-earth compounds have been the topic of growing interest recently. At low temperatures, dilute magnetic alloys show remarkable properties, which are mainly related to single-site Kondo effect. However, it has been noticed that even in the typical dilute magnetic alloys there are always traces of interimpurity correlations. These interimpurity correlations [22],[23] can lead to suppression of Kondo behaviour, formation of clusters, etc. In the systems that contains rare earth ions the specific low-temperature behaviour mainly shows the large conduction electron masses. For the heavy fermion systems the problem of interimpurity correlations is related to the understanding of their magnetic properties.
Very recently a new development in this field has emerged [14]-[28] which is related to alloy systems in which radical changes in physical properties occur with relatively modest changes in chemical composition [136]–[138].
The formation of the singlet state for the single-impurity Anderson and Kondo problem is now well understood within the Bethe-Ansatz scheme. As for dynamical properties, even for single-impurity Anderson model, the problem is only partially understood at present. The including of interimpurity correlations [22],[23] makes the problem even more difficult. Of special interest is the unsolved problem of the reduced magnetic moment in Ce-based alloys and description the heavy fermion state in the presence of the coexisting magnetic state. In other words our main interest is the understanding of the competition of the Kondo screening and RKKY exchange interactions. Depending on the relative magnitudes of the Kondo temperature and RKKY exchange integral, materials with different characteristics are found, which are classified as non-magnetic and magnetic concentrated Kondo systems. The latter, *KONDO MAGNETS* are our main interest here. There are some experimental evidences [136],[138] that this magnetism is not that of a localized systems, but have some features of band magnetism [139]. This is very intriguing conjecture which need the very careful investigation [23].
It is worthy to underline that in spite many theoretical efforts, a comprehensive understanding of the heavy fermion phenomenon is still lacking. From the point of view of the experimentalist [140] the heavy fermion state is the heavy-electron Fermi-liquid state that occurs in the rare-earth anomalous compounds at low temperatures and is a consequence of the Kondo effect. The direct evidence for the existence of the heavy-fermion quasiparticles gives the observation of the de Haas - van Alphen effect, a periodic dependence of magnetic susceptibility on applied magnetic field. However, the recent investigations [14] give certain evidences for deviation from simple Fermi-liquid picture. Furthermore, there are effects which have very complicated and controversial origination. Let us consider the experimental investigation of the interesting alloy system $Ce(Ru_{1-x}Rh_x)_3B_2$, where the physical properties change from superconducting to ferromagnetic as x changes from 0 to 1. The ferromagnetism occurs in the range $0.84 \leq x \leq 1$. The maximal magnetic

transition temperature Tm = 113K. The observable averaged magnetic moment per site reduced strongly. In seeking to explain such anomalous magnetic behaviour, Allen et al [141] have proposed that the natural scenario for incorporating the Kondo effect in a ferromagnetic state is that of new notion, namely *Exchange Split Kondo Resonance*. This picture could also be described by saying that the ferromagnetic state is a band ferromagnet built from the quasiparticles of a Kondo Fermi liquid. The theory in this namely spirit has been proposed earlier by Grewe and Welslau [139]. The later theory is based on the periodic Anderson model(PAM). A ladder summation for the particle-hole propagator of the full interacting system, including local quasiparticle repulsion, leads to a Stoner-like expression for the magnetic susceptibility χ,

$$\chi(q,\omega) = \frac{\chi_0(\omega)}{1 - U_{QP} Q^{ph}_{QP}(q,\omega)}. \tag{12}$$

It is possible to represent this expression in another form [142](c.f. [23])

$$\chi^{-1}(q,\omega) = \chi_0^{-1}(q,\omega) - K(q,\omega,T). \tag{13}$$

The semi-qualitative analysis show that the contribution K can induce cooperative magnetic behaviour, either RKKY type or of a type which may be described as exchange splitting of heavy fermion bands.
It seems that alloy system $Ce(Cu_{1-x}Ni_x)_2Ge_2$ may be a good candidate for realization of this unusual *Heavy Fermion Band Magnet*. The neutron scattering investigations and combined measurements show the transition to incommensurate antiferromagnetic phase with reduced magnetic moment [136]. Furthermore, recently Steglich et al [138] have confirmed this statement and, additionally, have predicted HFBM-phase even for $CeCu_2Si_2$ at Tn = 0.6-0.8 K! This is very intriguing conjecture and confirm the Ott's remark about heavy fermions as "a lasting source of puzzles" [14]. Note, however that there are more sober opinion that at present time it cannot be completely excluded that the emergence of the tiny moment is related to metallurgical problems (defects etc) [143],[144].
The concrete pictures considers above may be far from being realistic but one has always to keep in mind that for both systems, HTSC and HF, we lack a theory which can treat consistently both strong and weak electron correlation and the spin and charge degrees of freedom. As regards to the relationship between the HTSC and HF, both these materials may have a magnetic (i.e. spin fluctuations [7]) mechanism that is responsible for the formation of the superconducting electron pairs. From the experimental point of view there are some common features of the both classes of the materials [145]. From the theoretical point of view [146] such common features more or less transparent. Indeed, the minimal version of the Emery model (3) correspond to the periodic Anderson model by the appropriate redefinition of the parameters. The magnitudes of the parameters tell us that the HTSC oxides correspond to the strong coupling Kondo regime of the Kondo lattice, whereas the HF correspond to the weak coupling Kondo regime. Unfortunately, our understanding of this interrelation are still qualitative, but this field are developing quickly [147].

7 Irreducible Green's Functions Method

In this Section, we discuss briefly the novel nonperturbative approach for description of the many-body dynamics of the Higly Correlated Systems. At this point it is worthwhile to underline that it is essential to apply an adequate method in order to solve a concrete physical problem; the final solution should contain a correct physical reasoning in a most natural way. The list of many-body techniques that have been applied to strongly correlated systems is extensive. The problem of adequate description of many-body dynamics for the case of very strong Coulomb correlations has been explicitly raised by Anderson, who put the direct question: "... whether a real many-body theory would give answers radically different from the Hartree-Fock results?" [148]. The formulation of the Anderson model and closely related Hubbard model [149] dates really a better understanding of the electronic correlation in solids, especially if the relevant electrons are modelled better by tight-binding approximation. Both of the models, Anderson and Hubbard, are often referred to as the simplest models of magnetic metals and alloys. This naive perception contradicts the enormous amount of theoretical papers which has been published during the last decades and devoted to attacking the Anderson and Hubbard models by many refined theoretical techniques. As is well known now, the simplicity of the Anderson/Hubbard models manifest itself in the dynamics of a two-particle scattering. Nevertheless, as to the true many-body dynamics, there is still no simple and compact description, except in a very few limiting cases. Quite recently, since the discovery of HTSC, many theoretical investigations on its mechanism have been done invoking the strongly correlated models [1]-[5]. In this Section it will be attempted to justify the use of a novel Irreducible Green's Function (IGF) approach [150]-[153]. A number of other approaches for the strongly correlated electronic systems have been proposed and the our approach is in many respect an additional and incorporate the logic of development of many-body techniques as was mentioned in Introduction.

Here I will outline my understanding of the problem of Strong correlation from the point of view of the many-body theorist [154]. Let me first sketch the logic of development of the many-body theory. The study of the quasiparticle excitations in solids has been one of the most fascinating subjects for many years. The considerable progress in studying the spectra of elementary excitations and thermodynamic properties of many-body systems has been for the most part due to the development of the temperature dependent Green's Functions method. We have developed the helpful reformulation of the two-time GF-method which is especially adjusted for the strongly correlated systems. The full problem cannot be handled and one makes the approximations. In our approach the approximations are introduced in a very systematic way on the basis of the concept of **"GENERALIZED MEAN FIELDS"**. These GMFs have a complicated structure for the strongly correlated case and are not reduced to the functional of the mean densities of the electrons. This is in short the thrill of our approach.

To clarify the foregoing, let us consider the retarded GF of the form

$$G^r(t,t') = \ll A(t), B(t') \gg = -i\theta(t-t') < [A(t)B(t')]_\eta >, \eta = \pm 1. \quad (14)$$

As an introduction of the concepts of IGFs let us describe the main ideas of this approach in a symbolic form. To calculate the retarded GF G(t - t') let us write down the equation

of motion for it:

$$\omega G(\omega) = < [A, A^+]_\eta > + \ll [A, H]_- | A^+ \gg_\omega . \quad (15)$$

The essence of the method is as follows [150]-[153]. It is based on the notion of the *"irreducible"* parts of GFs (or the irreducible parts of the operators, out of which the GF is constructed) in terms of which it is possible, without recourse to a truncation of the hierarchy of equations for the GFs, to write down the exact Dyson equation and to obtain an exact analytical representation for the self-energy operator. By definition we introduce the **irreducible** part (ir) of the GF

$$^{ir} \ll [A, H]_- | A^+ \gg = \ll [A, H]_- - zA | A^+ \gg . \quad (16)$$

The unknown constant z is defined by the condition (or constraint)

$$< [[A, H]_-^{ir}, A^+]_\eta > = 0. \quad (17)$$

From the condition (17) one can find:

$$z = \frac{< [[A, H]_-, A^+]_\eta >}{< [A, A^+]_\eta >} = \frac{M_1}{M_0}. \quad (18)$$

Here M_0 and M_1 are the zeroth and first order moments of the spectral density. Therefore, the irreducible GFs (16) are defined so that it cannot be reduced to the low-order ones by any kind of decoupling. It is worthy to note that the irreducible correlation functions are well known in statistical mechanics [152]. In the diagrammatic approach the irreducible vertices are defined as the graph that do not contain inner parts connected by the G^0 -line. With the aid of the definition (16) these concepts are translating into the language of retarded and advanced GFs. This procedure **extract all relevant** (for the problem under consideration) *mean field contributions* and puts them into the **generalized mean-field** GF, which here are defined as

$$G^0(\omega) = \frac{< [A, A^+]_\eta >}{(\omega - z)}. \quad (19)$$

To calculate the IGF $^{ir} \ll [A, H]_-(t), A^+(t') \gg$ in (15), we have to write the equation of motion after differentiation with respect to the second time variable t'. The condition (17) remove the inhomogeneous term from this equation. If one introduces an irreducible part for the right-hand side operator as discussed above for the "left" operator, the equation of motion (15) can be exactly rewritten in the following form

$$G = G^0 + G^0 P G^0. \quad (20)$$

The scattering operator P is given by

$$P = (M_0)^{-1} \, ^{ir} \ll [A, H]_- | [A^+, H]_- \gg^{ir} (M_0)^{-1}. \quad (21)$$

The structure of the equation (20) enables us to determine the self-energy operator M, in complete analogy with the diagram technique

$$P = M + M G^0 P. \quad (22)$$

Approximate solutions are constructed as definite approximations for the self-energy operator M, as defined by Eq.(22). Therefore, in contrast to the standard equation-of-motion approach the decoupling will be introduced in the self-energy operator only. It is important to stress here that this last point is a very strong feature of this method, because of we operate with correct functional structure for the single-particle GF, namely we can write down the formal solution of the Dyson equation in the form

$$G = [(G^0)^{-1} - M]^{-1}. \qquad (23)$$

The specific method of introducing irreducible parts of GFs (we may equivalently speak of irreducible operators) depends on the form of operator A, the type of Hamiltonian and the condition of the problem. The general philosophy of the IGF method lies in the separation and identification of elastic scattering effects and inelastic ones. This last point is quite often underestimated, since there are quite a lot of works where both effects are mixed. However, as far as the right definition of quasiparticle damping is concerned, the separation of elastic and inelastic scattering processes is believed to be crucial for many-body systems with complicated many-branch spectra and strong interaction [22],[111]–[113]. This field is too extended to be reviewed as a whole in the present context. The most important conclusion to be drawn from this Section is that the GMF, can have, in general, a very non-trivial structure.

The existing applications of the GFs method in the standard form for HTSC or HF are too crude (i.e. [155],[156]) and describe the strong Coulomb correlation in the "Hubbard I" approximation only. From the other hand, there are a few attempts [157],[158] to use the GFs technique in a more correct way, incorporating some ideas of the IGFs method. This way are more promising , but additional efforts in this direction should be done. We plan to look into this aspect of the problem in the future.

8 Concluding Remarks

To summarize the results reported here, we illustrate the fact that it is possible to construct realistic models which are suitable for describing, at least partly, the properties of the Highly Correlated Systems, such as HTSC and HF materials. It is shown that the spins and carriers in the copper oxides and heavy fermions are coupled in a very nontrivial way. The arguments which seem to support the spin-polaron pairing mechanism in the copper oxides have been presented. In order to get a more complete picture of the strong correlations in the HTSC and HF the useful complimentary approaches must be analyzed. The functional integration method [159], [160] and higher-dimensions studies certainly should be considered in this aspect. The progress is expected from the additional efforts which will use the various advanced methods of the quantum statistical mechanics and both numerical and analytical techniques to attack this fascinating and extremely difficult problem of the Strong Electron Correlation. We hope that our analysis may be useful in further studies of the role of the strong electron correlation in HTSC and HF. Much remains to be done before one may claim to have a fully settled theories of the both phenomena. Nevertheless, may be someone will propose in the near future the "crazy" idea, which will solve the problem of the strongly interacting fermions on a

lattice (c.f. [161]) in the unusually simple and compact way, in spite of famous remark of Lieb and Mattis , who claimed that this problem is the same difficulty as searches for "philosophical stone". We believe that the IGFs method gives some real insight into better understanding of the HCS namely in this sense! I would like to finish this tale story with the following citation from F.J.Dyson : "Thirty-one years ago, Dick Feynman told me about his 'sum over histories' version of quantum mechanics. **'The electron does anything it likes'**, he said. **'It goes in any direction at any speed, forward or backward in time, however it likes, and then you add up amplitudes and it gives you the wave-function '**. I said to him 'You are *crazy*'. **But he wasn't!"**

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