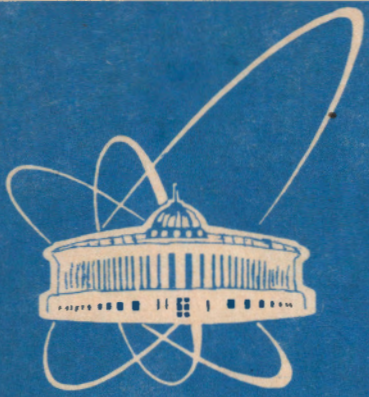

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E17-95-295

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ON THE DYNAMICAL SOLUTION OF THE ANDERSON MODEL

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1995

The problem of the adequate description of the strongly correlated electron systems has been studied intensively during the last decade, especialy in context of Heavy Fermions and High-Tc superconductivity [1]. The understanding of the true nature of the electronic states and their quasiparticle dynamics are the one of the central topics of the current experimental and theoretical efforts in the field. The plenty of experimental and theoretical results show that this many-body quasiparticle dynamics is quite non-trivial. The theoretical description of the strongly correlated systems have led to the formulation of two model Hamiltonians which plays a central role in our attempts to get an insight into this complicated problem. These are the Anderson single-impurity model(SIAM) [2] and Hubbard model [3]. It was only relatively recently recognized that the both model have a very complicated many-body dynamics and their "simplicity" manifests itself in the dynamics of two-particle scattering, as was shown via elegant Bethe-anzatz solution [4]. In this paper the problem of the adequate description of the many-body dynamics of SIAM will be discussed in the framework of equation-of-motion appproach for two-time thermodynamic Green's Functions. Our main motivation was the fact that the consistent theory of dynamical properties of the Hubbard model was formulated recently [5] using this approach. The second motivation was recent publication [6], where an "exact" dynamical solution of the SIAM has been derived by means the equation of motion for the two-time GFs. This "derivation" gives to us an opportunity to emphasize some important issues about the relevant dynamical solutions of the strongly correlated electron models (SIAM, Hubbard model, PAM etc.) and to formulate in a more sharp form the ideas of the method of the Irreducible Green's Functions (IGF) [7]. This IGF method allows one to describe the quasiparticle spectra with damping of the strongly correlated electron systems in a very general and natural way and to construct the relevant dynamical solution in a self-consistent way on the level of Dyson equation without decoupling the chain of the equation of motion for the GFs.

Let us consider standard Hamiltonian of SIAM [2]:

$$H = \sum_{k\sigma} \epsilon_k c^+_{k\sigma} c_{k\sigma} + \sum_{\sigma} E_{o\sigma} d^+_{o\sigma} d_{o\sigma} + U/2 \sum_{\sigma} n_{o\sigma} n_{o-\sigma} + \sum_{k\sigma} V_k (c^+_{k\sigma} d_{o\sigma} + d^+_{o\sigma} c_{k\sigma}) \quad (1)$$

where $c^+_{k\sigma}$ and $d^+_{o\sigma}$ are respectively the creation operators for conduction and localized electrons; other notations are standard. In the past years many theoretical papers have been published , in which the approximative dynamical solution of the model (1) have been investigated by means of various advanced methods of many-body theory. Despite the considerable contributions to development of the many-body theory and to our better understanding of the physics of the correlated electron systems, the fully consistent dynamical analytycal solution of the SIAM is still lacking. A detailed review of the results obtained thus far and the methods used will be done in an extended publication. Here we shall discuss some selected papers

only which are directly related to the problem under consideration [8] - [13]. Our goal is to propose the new nonperturbative many-body approach for description of the many-body dynamics of SIAM at finite temperatures using the circle of ideas of the Irreducible Green's Functions approach for the consideration of the strongly correlated electron systems [1], [5], [7]. The interplay and the competition of the kinetic energy (ϵ_k), potential energy (U) and hybridisation (V) affects substantially the electronic spectrum. Because these aspects of the problem are of great importance and are still not yet clarified completely(as it follows e.g. from paper [6]), we briefly discuss these questions here. The renormalized electron energies are temperature dependent and the electronic states have a finite life times. These effects are most suitable accounted for by the Green's functions method [14]. The purpose of the present approach is to find the electronic quasiparticle spectrum re-normalized by the interactions(U- and V-terms) in a wide temperature and parameters of the model range and to account explicitly for the contribution of damping of the electronic states when calculating the various characteristics of the SIAM.
For this aim we shall use the method of Irreducible Green's Functions (IGF) for the strongly correlated electronic systems [1], [5]. The essense of the methods is as follows [7].
The introduction of the irreducible parts of the GFs results in separation of all suitable renormalizations of the "generalized mean fields"(GMF). As a result, without having to make any truncation of the hierarchy of equations for the GFs, one can write down a Dyson equation (in terms of retarded GFs !)

$$G = G^{MF} + G^{MF} M G \tag{2}$$

and obtain an exact analytical representation for the self-energy operator M in terms of higher-order GFs

$$M = G^{-1} - (G^{MF})^{-1} \tag{3}$$

Approximate solutions are constructed as definite approximations for the self-energy, in another words on the level of the higher-order GFs. It is necessary to emphasize that there is an intimate connection between adequate introductions of mean fields and internal symmetries of the Hamiltonian. Though we do not want to go here into the mathematical subtleties of defining the correct mean fields for different models, we shall mention only that GMF can exhibit a quite non-trivial structure, especially for the strongly correlated case [5], [12]. To obtain this structure correctly, one must construct the full GF from the complete algebra of relevant operators.
The fundamental role of the relevant algebra of the operators has been discussed in papers [12], [13] , where the dynamical solution of SIAM, periodic Anderson model(PAM) and two-impurity Anderson model (TIAM) has been considered by the IGF method. The both weak and strong correlation limits have been considered. It was shown, using the minimal algebra of relevant operators, that the construction

of the GMFs for SIAM is quite non-trivial for the strongly correlated case and it is rather difficult to get it from an intuitive physical point of view.
In this papers we want to continue this line of consideration dealing with a more extended algebra of operators from which the relevant matrix GF will be constructing. In the same spirit it belongs to the most important intentions of this work to provide the basis for future consideration of the self-consistent interpolation solutions of SIAM and PAM which will be done in the more extended papers elsewhere.
At this point it is worthwhile to underline that despite that the fully consistent dynamical solution of SIAM is still lacking, a few important contributions has been done previously with the equations of motion for the GFs. To give a more instructive discussion let us consider the single- particle GF of localized electrons, which is defined as

$$G_\sigma(t) = << d_{o\sigma}(t), d^+_{o\sigma} >> = -i\theta(t) < [d_{o\sigma}(t), d^+_{o\sigma}]_+ > = 1/2\pi \int_{-\infty}^{+\infty} d\omega \exp(-i\omega t) G_\sigma(\omega) \tag{4}$$

In the important paper [8] the calculation of the GF (4) has been considered in the limit of infinitely strong Coulomb correlation U and small hybridisation V. It was shown, with the using the decoupling procedure for the higher-order GFs, that the obtained solution gives the correct result in the Kondo limit at low temperatures and for some other limits. The functional structure of the Lacroix's solution generalize the well known "interpolative", small-V, solution [9] of SIAM:

$$G_\sigma(\omega) = \frac{1 - < n_{o-\sigma} >}{\omega - E_{o\sigma} - S(\omega)} + \frac{< n_{o-\sigma} >}{\omega - E_{o\sigma} - S(\omega) - U} \tag{5}$$

where

$$S(\omega) = \sum_k \frac{|V_k|^2}{\omega - \epsilon_k} \tag{6}$$

This solution gives the correct results for $U = 0$ and $V = 0$ and is the simplest reasonable "atomic-like" solution of SIAM. This solution is valid at small V only. Oh and Doniach found [9] that for $V > 0.5$ eV , the spectral intensity of the GF (5) starts to go negative for a certain range of frequency values, indicating that their decoupling procedure does not conserve probability at each value of ω. To show this, let us remind how to get solution (5). It follows from the well known system of equation for small-V limit:

$$(\omega - E_{o\sigma} - S(\omega)) << d_{o\sigma} | d^+_{0\sigma} >>_\omega = 1 + U << d_{o\sigma} n_{o-\sigma} | d^+_{o\sigma} >>_\omega, \tag{7}$$

$$(\omega - E_{o\sigma} - U) << d_{o\sigma} n_{o-\sigma} | d^+_{o\sigma} >>_\omega \approx < n_{o-\sigma} > + \sum_k V_k << c_{k\sigma} n_{o\sigma} | d^+_{o\sigma} >>_\omega, \tag{8}$$

$$(\omega - \epsilon_k) << c_{k\sigma} n_{o-\sigma} | d^+_{o\sigma} >>_\omega = V_k << d_{o\sigma} n_{o-\sigma} | d^+_{o\sigma} >>_\omega \tag{9}$$

The equation (8) is approximative; it include two more terms, which were threated in the limit of small V in paper [8]. The solution (5) has been obtained in paper [6] and presented as an "exact". We shall see later on that, in fact, all results in [6] are approximative and are valid in the lowest order in V.
Another advanced many-body approach to analytical solution of SIAM was proposed in paper [10]. The Schwinger-type functional derivative technique has been used in [10] to get a solution, which have a number of truly remarkable properties. This solution was first found analytically [10], then only recently verified numerically [11]. To find more complex expansion, including both U and V, the "mean-fields" in paper [10] were introduced as follows:

$$\begin{aligned}
&<< d_{o\sigma} d^+_{o-\sigma} c_{k-\sigma} | d^+_{o\sigma} >> \approx < d^+_{o-\sigma} c_{k-\sigma} >< d_{o\sigma} | d^+_{o\sigma} >>, \\
&<< d_{o\sigma} c^+_{k-\sigma} d_{o-\sigma} | d^+_{o-\sigma} >> \approx < c^+_{k-\sigma} d_{o-\sigma} >< d_{o\sigma} | d^+_{o\sigma} >>, \\
&<< c_{k\sigma} d^+_{o-\sigma} c_{p-\sigma} | d^+_{o\sigma} >> \approx < d^+_{o-\sigma} c_{p-\sigma} >< c_{k\sigma} | d^+_{o\sigma} >>, \\
&<< c_{k\sigma} c^+_{p-\sigma} d_{o-\sigma} | d^+_{0\sigma} >> \approx < c^+_{p-\sigma} d_{o-\sigma} >< c_{k\sigma} | d^+_{o\sigma} >>
\end{aligned} \tag{10}$$

In fact, the procedure of introduction of the mean field corrections in the paper [10] remind (but not coincide) with that of the more systematic IGF method. The inelastic scattering corrections (self- energy) and elastic ones (mean-field) are separated in the IGF method in the most consistent and general way. The Neal's approximation (10) is valid also for the small V but, of course, completely in different sense that solution (5).
We now return to the IGF method again and consider how the computations of papers [12], [13] changes for more general algebra of operators. Our goal is to generalise solution (5) with IGF approach in a self-consistent way. In complete analogy with [12] let us consider the following equation of motion in the matrix form

$$\sum_p F(p,k) G_\sigma(p,\omega) = I + \sum_p V_p D(p,\omega) \tag{11}$$

where G is initial 4×4 matrix GF and D is the higher-order GF. We postpone to write down explicitly the relevant 16 GFs from which matrix GF G consist of till extended publication. For our aims here it will be enough to proceed forth in the following way. The equation (11) results from the first-time differentiation of the GF G and is a starting point for the IGF approach. If one introduces irreducible part for the higher-order GF D, by precisely the same steps as we have used in paper [12] and introduce the GMF GF according to

$$\sum_p F(p,k) G^{MF}_\sigma(p,\omega) = I, \tag{12}$$

then we will be able to write down explicitly the Dyson equation (3) and the exact

expression for the self-energy M in the matrix form:

$$M_\sigma(k,\omega) = I^{-1} \sum_{p,q} V_p V_q \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & M_{33} & M_{34} \\ 0 & 0 & M_{43} & M_{44} \end{pmatrix} I^{-1} \tag{13}$$

Here matrix I is given by

$$\begin{pmatrix} 1 & 0 & 0 & < n_{o-\sigma} > \\ 0 & 1 & < n_{o-\sigma} > & 0 \\ 0 & < n_{o-\sigma} > & < n_{o-\sigma} > & 0 \\ < n_{o-\sigma} > & 0 & 0 & < n_{o-\sigma} > \end{pmatrix}$$

and the the matrix elements of M have the form:

$$M_{33} = << A^{ir}_1(p) | B^{ir}_1(q) >>, M_{34} = << A^{ir}_1(p) | B^{ir}_2(k,q) >>$$

$$M_{43} = << A^{ir}_2(k,p) | B^{ir}_1(q) >>, M_{44} = << A^{ir}_2(k,p) | B^{ir}_2(k,q) >>$$

Since self-energy M describes the processes of inelastic scattering of electrons (c-c , d-d and c-d types), its approximate representation would be defined by the nature of the physical assumptions about this scattering.
To get an idea about the functional structure of our GMF solution (12) let us write down the matrix element G^{MF}_{33}:

$$G^{MF}_{33} = << d_{o\sigma} n_{o-\sigma} | d^+_{o\sigma} n_{o-\sigma} >> = \frac{< n_{o-\sigma} >}{\omega - E^{MF}_{o\sigma} - U - S^{MF}(\omega) - Y(\omega)} + \frac{< n_{o-\sigma} > Z(\omega)}{(\omega - E^{MF}_{o\sigma} - U - S^{MF}(\omega) - Y(\omega))(\omega - E_{o\sigma} - S(\omega))} \tag{14}$$

$$Y(\omega) = \frac{U Z(\omega)}{\omega - E_{o\sigma} - S(\omega)} \tag{15}$$

$$Z(\omega) = S(\omega) \sum_p \frac{V_P L_{41}}{\omega - \epsilon^{MF}_p} + \sum_p \frac{|V_p|^2 L^{42}}{\omega - \epsilon^{MF}_p} + S(\omega) L^{31} + \sum_p V_p L^{32} \tag{16}$$

Here the coefficients L^{41}, L^{42}, L^{31} and L^{32} are the certain complicated averages (c.f. [12]) from which the functional of the GMF is build.
We now return to a description of some of the issues involved in deciding whether or not the solution of paper [6] is "exact". For this reason we have tried in this paper to make our presentation of the Irreducible Green's Functions solution of SIAM as

concise as possible. From now on we shall concenrate only on the our first equation of motion (11) , before introducing the irreducible GFs. Let us put simply in this equation the higher-order GF $D = 0$! To distinguish this simplest equation from the GMF one (12) we write it in the following form

$$\sum_p F(p,k)G^0(p,\omega) = I \tag{17}$$

The corresponding matrix elements in which we are interesting in here reads

$$G^0_{22} = << d_{o\sigma}|d^+_{o\sigma} >>= \frac{1- < n_{o-\sigma} >}{\omega - E_{o\sigma} - S(\omega)} + \frac{< n_{o-\sigma} >}{\omega - E_{o\sigma} - S(\omega) - U} \tag{18}$$

$$G^0_{33} = << d_{o\sigma}n_{o-\sigma}|d^+_{o\sigma}n_{o-\sigma} >>= \frac{< n_{o-\sigma} >}{\omega - E_{o\sigma} - S(\omega) - U} \tag{19}$$

$$G^0_{32} = << d_{o\sigma}n_{o-\sigma}|d^+_{o\sigma} >>= G^0_{33} \tag{20}$$

The conclusion is rather evident. The results of paper [6] follows from our matrix GF (11) in the lowest order in V, even before introduction of GMF corrections, not speaking about of the self-energy corrections. The two GFs G^0_{32} and G^0_{33} are equal only in the lowest order in V. It is quite clear, that the full our solution, which includes the self-energy corrections, is much more complicated as well as the solutions of [8], [10]. In fact, it is very easy to rewrite the system of the equations of motion (2) - (4) of paper [6] in the following equivalent form

$$<< d_{o\sigma}|d^+_{o\sigma} >>= g^0 + g^0 P g^0 \tag{21}$$

$$g^0 = (\omega - E_{o\sigma} - S(\omega))^{-1} \tag{22}$$

$$P = U < n_{o-\sigma} > + U^2 << d_{o\sigma}n_{o-\sigma}|d^+_{o\sigma}n_{o-\sigma} >>_\omega \tag{23}$$

This equation has been derived and used in paper [12]. The advantage of the equation (21) is that it is purely identity and does not include any approximation. If we insert our GMF solution (14) in (21) we shall get an essentially new dynamical solution of SIAM which reproduces the exact solutions of SIAM for $V = 0$ and $U = 0$ and generalise (even on the mean-field level) the solutions of papers [8], [10]. The identity (21) permit also to reformulate the problem of the derivation of the suitable interpolative solution of the SIAM, including the U-perturbation expansion, on the rather different then the single-particle GF level, on the level of the higher-order GFS as it will be shown in a separate publication.
It is worthwhile to underline that our 4×4 matrix GMF GF (12) gives only approximative description of the suitable mean fields. If we shall consider more extended 8×8 algebra, we shall get the more correct structure of the relevant GMF. A more rigorous derivation of this relevant algebra, showing its central importance for the self-consistent dynamical solution ot SIAM, will be presented elsewhere.

In summary, we presented in this paper a general technique how a dynamical solution for SIAM at finite temperatures and for the broad interval of the values of the model parameters can be constructed in the spirit of Irreducible Green's Function approach. We used an exact result to connect the single-particle GF with the higher-order GF to obtain an complex expansion in terms of U and V for the propagator. This approach offer a new way for the systematic constructions of the approximative dynamical solutions of SIAM, PAM and other models of the strongly correlated electron systems. The work in this direction is in progress.

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Received by Publishing Department
on July 7, 1995.