

# Electronic Dynamics of the Anderson Model. The Many-Body Approach

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## Abstract

A review of electronic dynamics of single-impurity and many-impurity Anderson models is contained in this report. Those models are used widely for many of the applications in diverse fields of interest, such as surface physics, theory of chemisorption and adsorbate reactions on metal surfaces, physics of intermediate valence systems, theory of heavy fermions, physics of quantum dots and other nanostructures. While standard treatments are generally based on perturbation methods, our approach is based on the non-perturbative technique for the thermodynamic Green functions. The method of the irreducible Green functions is used as the basic tool. This irreducible Green functions 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 equations of motion for the Green functions. The subject matter includes the improved interpolating solution of the Anderson model. It was shown that an interpolating approximation, which simultaneously reproduces the weak-coupling limit up to second order in the interaction strength  $U$  and the strong-coupling limit up to second order in the hybridization  $V$  (and thus also fulfils the atomic limit) can be formulated self-consistently. This approach offers a new way for the systematic construction of approximate interpolation dynamical solutions of strongly correlated electron systems.

**Keywords:** Many-particle interacting systems; statistical physics; physical chemistry; surface physics; theory of chemisorption; fundamental aspects of catalysis; hybridizing localized and itinerant electrons; the single-impurity, two-impurity and periodic Anderson model; the electronic quasiparticle dynamics; the Green functions approach; Dyson equation; quasiparticle damping.

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# Contents

<b>1</b>	<b>Introduction</b>	<b>2</b>
<b>2</b>	<b>Hamiltonian of the Models</b>	<b>3</b>
2.1	Single-impurity Anderson model (SIAM) . . . . .	3
2.2	Periodic Anderson Model (PAM) . . . . .	3
2.3	Two-Impurity Anderson Model (TIAM) . . . . .	4
<b>3</b>	<b>The Method of Irreducible Green Functions</b>	<b>5</b>
<b>4</b>	<b>The Irreducible Green Functions Method and SIAM</b>	<b>7</b>
<b>5</b>	<b>SIAM. Strong Correlation</b>	<b>10</b>
<b>6</b>	<b>IGF Method and Interpolation Solution of SIAM</b>	<b>11</b>
<b>7</b>	<b>Quasiparticle Dynamics of SIAM</b>	<b>14</b>
<b>8</b>	<b>Complex Expansion for a Propagator</b>	<b>15</b>
<b>9</b>	<b>The Improved Interpolative Treatment of SIAM</b>	<b>17</b>
<b>10</b>	<b>Quasiparticle Many-Body Dynamics of PAM</b>	<b>21</b>
<b>11</b>	<b>Quasiparticle Many-Body Dynamics of TIAM</b>	<b>23</b>
<b>12</b>	<b>Conclusions</b>	<b>25</b>

# 1 Introduction

In this review we discuss the many-body quasiparticle dynamics of the Anderson impurity model<sup>1,2</sup> and its generalizations<sup>3</sup> in the framework of the equation-of-motion method<sup>4,5,6,7,8,9,10,11,12</sup> at finite temperatures.

The studies of strongly correlated electrons in solids and their quasiparticle dynamics are intensively explored subjects in solid state physics.<sup>5,13,14,15</sup> Electronic dynamics in the bulk and at the surface of solid materials are well known to play a key role in a variety of physical and chemical phenomena.<sup>5,15,16,17,18,19,20</sup> One of the main aspects of such studies is the interaction of low-energy electrons with solids, where the calculations of inelastic lifetimes of both low-energy electrons in bulk materials and image-potential states at metal surfaces are highly actual problems. The calculations of inelastic lifetimes was made as a rule in a model of the homogeneous electron gas,<sup>15</sup> by using various approximate representations of the electronic response of the medium. Band-structure calculations, which have been carried out in literature may give a partial information only.

The band-structure approach<sup>14,21,22,23</sup> suffers from well known limitations. It cannot be validated in full measure in the case of very narrow bands and strongly correlated localized electrons.<sup>5,24,25</sup> An alternative approach is connected with using correlated fermion lattice models, like Anderson<sup>1,2</sup> and Hubbard model.<sup>26,27,28,29,30,31,32,33,34</sup>

The principal importance of this approach is related with the *dual character* of electrons in dilute magnetic alloys,<sup>35,36,37,38,39,40</sup> in transition metal oxides,<sup>5,41,42,43,44,45,46,47,48,49,50</sup> intermediate-valence solids,<sup>51,52,53</sup> heavy fermions,<sup>9,51,54,55,56</sup> high- $T_c$  superconductors,<sup>9,57</sup> etc. In these materials electrons exhibit both localized and delocalized features.<sup>5,41</sup> For example in paper<sup>53</sup> the electronic structure in solid phases of plutonium was discussed. The electrons in the outermost orbitals of plutonium show qualities of both *atomic* and *metallic* electrons. The metallic aspects of electrons and the electron duality that effect the electronic, magnetic and other properties of elements were manifested clearly.

The basic models to describe correlated electron systems are the single-impurity Anderson model (SIAM),<sup>1,2,35,56,58,59</sup> periodic Anderson model (PAM)<sup>60</sup> and the Hubbard model which exhibit the key physical feature, i.e., the competition between kinetic energy (itinerant) and potential energy (localized) effects.<sup>5,41,42</sup>

Indeed, the standard approach which is valid mainly for the simple and noble metals is provided by the band theory formalism for the calculation of the electronic structure of solids. For a better understanding of how structure and properties of solids may be related the chemically insightful concept of orbital interaction and the essential machinery of band theory should be taken into account<sup>25</sup> to reveal links between the crystal and electronic structure of periodic systems. In such a way, it was possible shown<sup>25</sup> how important tools for understanding properties of solids like the density of states, the Fermi surface etc., can be qualitatively formulated and used to rationalize experimental observations. It was shown that extensive use of the orbital interaction approach appears to be a very efficient way of building bridges between physically and chemically based notions to understand the structure and properties of solids.

The Anderson and Hubbard models found a lot of applications in studies of surface physics,<sup>16,19</sup> theory of chemisorption and adsorption<sup>61,62,63,64,65</sup> and various aspects of physics of quantum dots.<sup>66,67,68,69,70,71,72,73,74,75,76,77</sup> However in spite of many theoretical efforts a fully satisfactory solution of the dynamical problem is still missing. The Bethe-ansatz solution of the SIAM allows for the determination of the ground state and thermodynamic static properties, but it does not allow for a determination of the dynamical properties. For their understanding the development of improved and reliable approximations is still justified and desirable. In this context it is of interest to consider an interpolating and improved interpolating approximations which were

proposed in the papers.<sup>6,7,8,9,10,11,12</sup> We will show that a self-consistent approximation for the SIAM can be formulated which reproduces all relevant exactly solvable limits and interpolates between the strong- and weak-coupling limit.

In connection with the dynamical properties the one-particle Green function is the basic quantity to be calculated. Subject of this survey is primarily devoted to the analysis of the relevant many-body dynamic solution of the single impurity Anderson model and its *correct functional structure*. We wish to emphasize that the correct functional structure actually arises both from the self-consistent many-body approach and intrinsic nature of the model itself. The important representative quantity is the *spectral intensity* of the Green function at low energy and low temperature. Hence, it is desirable to have a consistent and closed analytic representation for the one-particle Green function of SIAM. The papers<sup>6,7,8,9,10,11,12</sup> clearly show the importance of the calculation of the Green function and spectral densities for SIAM and the many-impurity Anderson model in a self-consistent way.

In this terse overview the problem of consistent analytic description of the many-body dynamics of SIAM is analyzed in the framework of the equation-of-motion approach for double-time thermodynamic Green functions.<sup>4,5</sup> In addition to the irreducible Green functions (IGF) approach,<sup>32,78,79,80,81,82,83,84,85</sup> we use a new **exact identity**,<sup>7,11,81</sup> relating the one-particle and many-particle Green functions. Using this identity, it was possible to formulate a consistent and general scheme for construction of generalized solutions of the Anderson model. A new approach for the complex expansion for the single-particle propagator in terms of Coulomb repulsion  $U$  and hybridization  $V$  is discussed as well. Using the exact identity, an essentially new many-body dynamic solution of SIAM was derived.

## 2 Hamiltonian of the Models

### 2.1 Single-impurity Anderson model (SIAM)

The Hamiltonian of the SIAM can be written in the form

$$H = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} + \sum_{\sigma} E_{0\sigma} f_{0\sigma}^\dagger f_{0\sigma} + \frac{U}{2} \sum_{\sigma} f_{0\sigma}^\dagger f_{0\sigma} f_{0-\sigma}^\dagger f_{0-\sigma} + \sum_{\vec{k}\sigma} V_{\vec{k}} (c_{\vec{k}\sigma}^\dagger f_{0\sigma} + f_{0\sigma}^\dagger c_{\vec{k}\sigma}), \quad (1)$$

where  $c_{\vec{k}\sigma}^\dagger$  and  $f_{0\sigma}^\dagger$  are the creation operators for conduction and localized electrons;  $\epsilon_{\vec{k}}$  is the conduction electron dispersion,  $E_{0\sigma}$  is the localized (f-) electron energy level and  $U$  is the intra-atomic Coulomb interaction at the impurity site.  $V_{\vec{k}}$  represents the  $s - f$  hybridization. In the following consideration we will omit the vector notation for the sake of brevity.

### 2.2 Periodic Anderson Model (PAM)

Let us now consider a lattice generalization of SIAM, the so-called periodic Anderson model (PAM). The basic assumption of the periodic impurity Anderson model is the presence of two well-defined subsystems, i.e. the Fermi sea of nearly free conduction electrons and the localized impurity orbitals embedded into the continuum of conduction electron states (in rare-earth compounds, for instance, the continuum is actually a mixture of  $s$ ,  $p$ , and  $d$  states, and the localized orbitals are

$f$  states). The simplest form of PAM

$$H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{i\sigma} E_0 f_{i\sigma}^\dagger f_{i\sigma} + U/2 \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} + \frac{V}{\sqrt{N}} \sum_{ik\sigma} (\exp(ikR_i) c_{k\sigma}^\dagger f_{i\sigma} + \exp(-ikR_i) f_{i\sigma}^\dagger c_{k\sigma}) \quad (2)$$

assumes a one-electron energy level  $E_0$ , hybridization interaction  $V$ , and the Coulomb interaction  $U$  at each lattice site. Using the transformation

$$c_{k\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_j \exp(-ikR_j) c_{j\sigma}^\dagger; \quad c_{k\sigma} = \frac{1}{\sqrt{N}} \sum_j \exp(ikR_j) c_{j\sigma} \quad (3)$$

the Hamiltonian (2) can be rewritten in the Wannier representation:

$$H = \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} E_0 f_{i\sigma}^\dagger f_{i\sigma} + U/2 \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} + V \sum_{i\sigma} (c_{i\sigma}^\dagger f_{i\sigma} + f_{i\sigma}^\dagger c_{i\sigma}). \quad (4)$$

If one retains the  $k$ -dependence of the hybridization matrix element  $V_k$  in (4), the last term in the PAM Hamiltonian describing the hybridization interaction between the localized impurity states and extended conduction states and containing the essence of a specificity of the Anderson model, is as follows

$$\sum_{ij\sigma} V_{ij} (c_{i\sigma}^\dagger f_{i\sigma} + f_{i\sigma}^\dagger c_{i\sigma}); \quad V_{ij} = \frac{1}{N} \sum_k V_k \exp[ik(R_j - R_i)]. \quad (5)$$

The on-site hybridization  $V_{ii}$  is equal to zero for symmetry reasons. Hence the Hamiltonian of PAM in the Bloch representation takes the form

$$H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{i\sigma} E_k f_{i\sigma}^\dagger f_{i\sigma} + U/2 \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} + \sum_{k\sigma} V_k (c_{k\sigma}^\dagger f_{k\sigma} + f_{k\sigma}^\dagger c_{k\sigma}). \quad (6)$$

Note that as compared to the SIAM, the PAM has its own specific features. This can lead to peculiar magnetic properties for concentrated rare-earth systems where the criterion for magnetic ordering depends on the competition between indirect RKKY-type interaction<sup>13</sup> (not included into SIAM) and the Kondo-type singlet-site screening (contained in SIAM).

The inclusion of inter-impurity correlations makes the problem even more difficult. Since these inter-impurity effects play an essential role in physical behaviour of real systems,<sup>8,81</sup> it is instructive to consider the two-impurity Anderson model (TIAM) too.

### 2.3 Two-Impurity Anderson Model (TIAM)

The two-impurity Anderson model was considered by Alexander and Anderson.<sup>3</sup> They put forward a theory which introduces the impurity-impurity interaction within a game of parameters.

The Hamiltonian of TIAM reads

$$H = \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i=1,2\sigma} E_{0i} f_{i\sigma}^\dagger f_{i\sigma} + U/2 \sum_{i=1,2\sigma} n_{i\sigma} n_{i-\sigma} + \sum_{i\sigma} (V_{ki} c_{i\sigma}^\dagger f_{i\sigma} + V_{ik} f_{i\sigma}^\dagger c_{i\sigma}) + \sum_{\sigma} (V_{12} f_{1\sigma}^\dagger f_{2\sigma} + V_{21} f_{2\sigma}^\dagger f_{1\sigma}) \quad (7)$$

where  $E_{0i}$  are the position energies of localized states (for simplicity, we consider identical impurities and  $s$ -type i.e. non-degenerate) orbitals:  $E_{01} = E_{02} = E_0$ . The hybridization matrix element  $V_{ik}$  was discussed in detail in Ref.<sup>8</sup> As for the TIAM, the situation with the right definition of the parameters  $V_{12}$  and  $V_{ik}$  is not very clear. The definition of  $V_{12}$  in<sup>3</sup> is the following:

$$V_{12} = V_{21}^\dagger = \int \phi_1^\dagger(\vec{r}) H_f \phi_2(\vec{r}) dr. \quad (8)$$

Note that  $H_f$  is without "H-F" (Hartree-Fock) mark. The essentially local character of the Hamiltonian  $H_f$  clearly shows that  $V_{12}$  describes the direct coupling between nearest neighboring sites (for a detailed discussion see Ref.<sup>8</sup> where the hierarchy of the Anderson models was discussed too).

### 3 The Method of Irreducible Green Functions

When working with infinite hierarchies of equations for Green functions<sup>4,5</sup> the main problem is finding the methods for their efficient decoupling, with the aim of obtaining a closed system of equations, which determine the Green functions. In the papers<sup>32,78,79,80,81</sup> devoted to studies of lattice systems of interacting fermions it was shown that for a wide range of problems in statistical mechanics<sup>82,83,84,85</sup> and theory of condensed matter one can outline a fairly systematic recipe for constructing approximate solutions in the framework of *irreducible Green functions* method. Within this approach one can look from a unified point of view at the main problems of fundamental characters arising in the method of two-time temperature Green functions.

The method of irreducible Green functions is a useful reformulation of the ordinary Bogoliubov-Tyablikov method of equations of motion.<sup>4,5</sup> The constructive idea can be summarized as follows. During calculations of single-particle characteristics of the system (the spectrum of quasiparticle excitations, the density of states, and others) it is convenient to begin from writing down Green function as a formal solution of the Dyson equation. This will allow one to perform the necessary decoupling of many-particle correlation functions in the mass operator. This way one can control the decoupling procedure conditionally, by analogy with the diagrammatic approach. In this approach the infinite hierarchy of coupled equations for correlation functions is reduced to a few relatively simple equations that effectively take into account the essential information on the system under consideration, which determine the special features of this concrete problem.

It is necessary to stress that the structure of solutions obtained in the framework of irreducible Green functions method is very sensitive to the order of equations for Green functions<sup>81</sup> in which irreducible parts are separated. This in turn determines the character of the approximate solutions constructed on the basis of the exact representation.

Now we introduce the retarded, advanced, and causal Green function:

$$G^r(A, B; t - t') = \langle \langle A(t), B(t') \rangle \rangle^r = -i\theta(t - t') \langle [A(t), B(t')]_\eta \rangle, \quad \eta = \pm, \quad (9)$$

$$G^a(A, B; t - t') = \langle \langle A(t), B(t') \rangle \rangle^a = i\theta(t' - t) \langle [A(t), B(t')]_\eta \rangle, \quad \eta = \pm, \quad (10)$$

$$G^c(A, B; t - t') = \langle \langle A(t), B(t') \rangle \rangle^c = iT \langle A(t) B(t') \rangle = i\theta(t - t') \langle A(t) B(t') \rangle + \eta i\theta(t' - t) \langle B(t') A(t) \rangle, \quad \eta = \pm. \quad (11)$$

Here  $\langle \dots \rangle$  is the average over the grand canonical ensemble,  $\theta(t)$  is the Heaviside step function; the square brackets denote either commutator or anticommutator ( $\eta = \pm$ ):

$$[A, B]_{-\eta} = AB - \eta BA. \quad (12)$$

An important ingredient for Green function application is their temporal evolution. In order to derive the corresponding evolution's equation, one has to differentiate Green function over one of

its arguments. In order to clarify the above general description, let us consider the equations of motion for the retarded Green function of the form  $\langle\langle A(t), A^\dagger(t') \rangle\rangle$

$$\omega G(\omega) = \langle[A, A^\dagger]_\eta\rangle + \langle\langle[A, H]_- | A^\dagger \rangle\rangle_\omega. \quad (13)$$

The irreducible (**ir**) Green function is defined by

$${}^{(ir)}\langle\langle[A, H]_- | A^\dagger \rangle\rangle = \langle\langle[A, H]_- - zA | A^\dagger \rangle\rangle. \quad (14)$$

The unknown constant  $z$  is found from the condition

$$\langle\langle{}^{(ir)}[A, H]_-, A^\dagger \rangle\rangle_\eta = 0. \quad (15)$$

It is worth noting that instead of finding the irreducible part of Green function

$${}^{(ir)}\langle\langle[A, H]_- | A^\dagger \rangle\rangle, \quad (16)$$

one can absolutely equivalently consider *the irreducible operators*

$${}^{(ir)}[A, H]_- \equiv ([A, H]_-)^{(ir)}. \quad (17)$$

Therefore, we will use both the notation  $({}^{(ir)}\langle\langle A|B \rangle\rangle)$  and  $\langle\langle(A)^{(ir)}|B \rangle\rangle)$ , whichever is more convenient and compact. Equation (15) implies

$$z = \frac{\langle\langle[A, H]_-, A^\dagger \rangle\rangle_\eta}{\langle[A, A^\dagger]_\eta\rangle} = \frac{M_1}{M_0}. \quad (18)$$

Here,  $M_0$  and  $M_1$  are the zero and first moments of the spectral density.<sup>4,5</sup> Green function is called **irreducible** (i.e. impossible to reduce to a desired, simpler, or smaller form or amount) if it cannot be turned into a lower order Green function via decoupling. The well-known objects in statistical physics are irreducible correlation functions. In the framework of the diagram technique the irreducible vertices are a set of graphs, which cannot be cut along a single line. The definition (14) translates these notions to the language of retarded and advanced Green functions. We attribute all the mean-field renormalizations that are separated by Eq. (14) to Green function within a *generalized mean field* approximation

$$G^0(\omega) = \frac{\langle[A, A^\dagger]_\eta\rangle}{(\omega - z)}. \quad (19)$$

For calculating Green function (14),  $({}^{(ir)}\langle\langle[A, H]_-(t), A^\dagger(t') \rangle\rangle)$ , we make use of differentiation over the second time  $t'$ . Analogously to Eq. (14) we separate the irreducible part from the obtained equation and find

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

Here, we introduced the scattering operator

$$P = (M_0)^{-1} \left( \langle\langle([A, H]_-)^{(ir)} | ([A^\dagger, H]_-)^{(ir)} \rangle\rangle \right) (M_0)^{-1}. \quad (21)$$

In complete analogy with the diagram technique one can use the structure of Eq. (20) to define the mass operator  $M$ :

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

As a result we obtain the exact Dyson equation (we did not perform any decoupling yet) for two-time temperature Green functions:

$$G = G^0 + G^0 M G. \quad (23)$$

According to Eq.(22), the mass operator  $M$  (also known as the self-energy operator) can be expressed in terms of the **proper** (called *connected* within the diagram technique) part of the many-particle irreducible Green function. This operator describes inelastic scattering processes, which lead to damping and to additional renormalization of the frequency of self-consistent quasi-particle excitations. One has to note that there is quite a subtle distinction between the operators  $P$  and  $M$ . Both operators are solutions of two different integral equations given by Eqs. (22) and (23), respectively. However, only the Dyson equation (23) allows one to write down the following formal solution for the Green function:

$$G = [(G^0)^{-1} - M]^{-1}. \quad (24)$$

This fundamental relationship can be considered as an alternative form of the Dyson equation, and as the **definition** of the mass operator under the condition that the Green function within the generalized mean-field approximation,  $G^0$ , was appropriately defined using the equation

$$G^0 G^{-1} + G^0 M = 1. \quad (25)$$

In contrast, the operator  $P$  does not satisfy Eq. (25). Instead we have

$$(G^0)^{-1} - G^{-1} = P G^0 G^{-1}. \quad (26)$$

Thus, it is **the functional structure** of Eq. (24) that determines the essential differences between the operators  $P$  and  $M$ . To be absolutely precise, the definition (22) has a symbolic character. It is assumed there that due to the similar structure of equations (9) - (12) defining all three types of Green functions, one can use the causal Green functions at all stages of calculation, thus confirming the sensibility of the definition (22). Therefore, one should rather use the phrase "an analogue of the Dyson equation". Below we will omit this stipulation, because it will not lead to misunderstandings. One has to stress that the above definition of irreducible parts of the Green function (irreducible operators) is nothing but a general scheme. The specific way of introducing the irreducible parts of the Green function depends on the concrete form of the operator  $A$  on the type of the Hamiltonian, and on the problem under investigation.

Thus, we managed to reduce the derivation of the complete Green function to calculation of the Green function in the generalized mean-field approximation and with the generalized mass operator. The essential part of the above approach is that the approximate solutions are constructed not via decoupling of the equation-of-motion hierarchy, but via choosing the functional form of the mass operator in an appropriate self-consistent form. That is, by looking for approximations of the form  $M \approx F[G]$ . Note that the exact functional structure of the one-particle Green function (24) is preserved in this approach, which is quite an essential advantage in comparison to the standard decoupling schemes.

## 4 The Irreducible Green Functions Method and SIAM

After discussing some of the basic facts about the correct functional structure of the relevant dynamic solution of correlated electron models we are looking for, described in previous Chapter, we give a similar consideration for SIAM. It was shown in Refs.,<sup>7,10,11,8</sup> using the minimal algebra of relevant operators, that the construction of the generalized mean fields for SIAM is quite



nontrivial for the strongly correlated case, and it is rather difficult to get it from an intuitive physical point of view.

To proceed let us consider first the following matrix Green function

$$\hat{G}(\omega) = \begin{pmatrix} \langle\langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle c_{k\sigma} | f_{0\sigma}^\dagger \rangle\rangle \\ \langle\langle f_{0\sigma} | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle f_{0\sigma} | f_{0\sigma}^\dagger \rangle\rangle \end{pmatrix}. \quad (27)$$

Performing the first-time differentiation and defining the irreducible Green function

$$\begin{aligned} {}^{(ir)}\langle\langle f_{0\sigma} f_{0-\sigma}^\dagger f_{0-\sigma} | f_{0\sigma}^\dagger \rangle\rangle_\omega &= \langle\langle f_{0\sigma} f_{0-\sigma}^\dagger f_{0-\sigma} | f_{0\sigma}^\dagger \rangle\rangle_\omega - \\ &\quad - \langle n_{0-\sigma} \rangle \langle\langle f_{0\sigma} | f_{0\sigma}^\dagger \rangle\rangle_\omega, \end{aligned} \quad (28)$$

we obtain the following equation of motion in the matrix form

$$\sum_p \hat{F}_p(\omega) \hat{G}_p(\omega) = \hat{1} + U \hat{D}^{(ir)}(\omega), \quad (29)$$

where all definitions are rather evident. Proceeding further with the IGF technique, the equation of motion (29) may be rewritten exactly in the form of the Dyson equation

$$\hat{G}(\omega) = \hat{G}^0(\omega) + \hat{G}^0(\omega) \hat{M}(\omega) \hat{G}(\omega). \quad (30)$$

The generalized mean field Green function  $G^0$  is defined by

$$\sum_p F_p(\omega) G_p^0(\omega) = \hat{I}. \quad (31)$$

The explicit solutions for diagonal elements of  $G^0$  are

$$\langle\langle f_{0\sigma} | f_{0\sigma}^\dagger \rangle\rangle_\omega^0 = \left( \omega - E_{0\sigma} - U n_{-\sigma} - S(\omega) \right)^{-1} \quad (32)$$

$$\langle\langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle_\omega^0 = \left( \omega - \epsilon_k - \frac{|V_k|^2}{\omega - E_{0\sigma} - U n_{-\sigma}} \right)^{-1}, \quad (33)$$

where

$$S(\omega) = \sum_k \frac{|V_k|^2}{\omega - \epsilon_k}. \quad (34)$$

The mass or self-energy operator, which describes inelastic scattering processes, has the following matrix form

$$\hat{M}(\omega) = \begin{pmatrix} 0 & 0 \\ 0 & M_{0\sigma} \end{pmatrix}, \quad (35)$$

where

$$M_{0\sigma} = U^2 \left( {}^{(ir)}\langle\langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle\rangle_\omega^{(ir)} \right)^{(p)}. \quad (36)$$

From the formal solution of the Dyson equation (30) one obtains

$$\langle\langle f_{0\sigma} | f_{0\sigma}^\dagger \rangle\rangle_\omega = \left( \omega - E_{0\sigma} - U n_{-\sigma} - M_{0\sigma} - S(\omega) \right)^{-1} \quad (37)$$

$$\langle\langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle_\omega = \left( \omega - \epsilon_k - \frac{|V_k|^2}{\omega - E_{0\sigma} - U n_{-\sigma} - M_{0\sigma}} \right)^{-1}. \quad (38)$$

To calculate the self-energy in a self-consistent way, we have to approximate it by lower-order Green functions. Let us start by analogy with the Hubbard model with a pair-type approximation<sup>32,79,81</sup>

$$M_{0\sigma}(\omega) = U^2 \int \frac{d\omega_1 d\omega_2 d\omega_3}{\omega + \omega_1 - \omega_2 - \omega_3} \times \quad (39)$$

$$[n(\omega_2)n(\omega_3) + n(\omega_1)(1 - n(\omega_2) - n(\omega_3))]g_{0-\sigma}(\omega_1)g_{0\sigma}(\omega_2)g_{0-\sigma}(\omega_3),$$

where we used the notation

$$g_{0\sigma}(\omega) = -\frac{1}{\pi} \text{Im} \langle \langle f_{0\sigma} | f_{0\sigma}^\dagger \rangle \rangle_\omega. \quad (40)$$

The equations (30) and (39) constitute a closed self-consistent system of equations for the single-electron Green function for SIAM model, but only for weakly correlated case. In principle, we can use, on the r.h.s. of Eq.(39), any workable first iteration-step form of the Green function and find a solution by repeated iteration. If we take for the first iteration step the expression

$$g_{0\sigma}(\omega) \approx \delta(\omega - E_{0\sigma} - Un_{-\sigma}), \quad (41)$$

we get, for the self-energy, the explicit expression

$$M_{0\sigma}(\omega) = U^2 \frac{n(E_{0\sigma} + Un_{-\sigma})(1 - n(E_{0\sigma} + Un_{-\sigma}))}{\omega - E_{0\sigma} - Un_{-\sigma}} \quad (42)$$

$$= U^2 Q_{-\sigma}(1 - Q_{-\sigma})G_\sigma^0(\omega),$$

where

$$Q_{-\sigma} = n(E_{0\sigma} + Un_{-\sigma}), \quad n(E) = \{\exp[(E - \mu)/k_B T] + 1\}^{-1}. \quad (43)$$

This is the well-known *atomic limit* of the self-energy.<sup>7,10,11,8</sup>

Let us try again another type of the approximation for  $M$ . The approximation which we will use reflects the interference between the one-particle branch and the collective one

$$\langle f_{0\sigma}(t)f_{0-\sigma}^\dagger(t)f_{0-\sigma}(t)f_{0-\sigma}^\dagger f_{0-\sigma}f_{0\sigma}^\dagger \rangle^{(ir)} \approx$$

$$\langle f_{0\sigma}^\dagger(t)f_{0\sigma} \rangle \langle n_{0-\sigma}(t)n_{0-\sigma} \rangle +$$

$$\langle f_{0-\sigma}^\dagger(t)f_{0-\sigma} \rangle \langle f_{0-\sigma}^\dagger(t)f_{0\sigma}(t)f_{0\sigma}^\dagger f_{0-\sigma} \rangle +$$

$$\langle f_{0-\sigma}^\dagger(t)f_{0-\sigma} \rangle \langle f_{0-\sigma}(t)f_{0\sigma}(t)f_{0\sigma}^\dagger f_{0-\sigma}^\dagger \rangle. \quad (44)$$

If we retain only the first term in (44) and make use of the same iteration as in (41), we obtain

$$M_{0\sigma}(\omega) \approx U^2 \frac{(1 - n(E_{0\sigma} + Un_{-\sigma}))}{\omega - E_{0\sigma} - Un_{-\sigma}} \langle n_{0-\sigma}n_{0-\sigma} \rangle. \quad (45)$$

If we retain the second term in (44), we obtain

$$M_{0\sigma}(\omega) = U^2 \int_{-\infty}^{+\infty} d\omega_1 d\omega_2 \frac{1 + N(\omega_1) - n(\omega_2)}{\omega - \omega_1 - \omega_2} \times$$

$$\left( -\frac{1}{\pi} \text{Im} \langle \langle S_0^\pm | S_0^\mp \rangle \rangle_{\omega_1} \right) \left( -\frac{1}{\pi} \text{Im} \langle \langle f_{0\sigma} | f_{0\sigma}^\dagger \rangle \rangle_{\omega_2} \right), \quad (46)$$

where the following notation were used:

$$S_0^+ = f_{0\uparrow}^\dagger f_{0\downarrow}; \quad S_0^- = f_{0\downarrow}^\dagger f_{0\uparrow}. \quad (47)$$

It is possible now to rewrite (46) in a more convenient way

$$M_{0\sigma}(\omega) = U^2 \int d\omega' \left( \cot \frac{\omega - \omega'}{2T} + \tan \frac{\omega'}{2T} \right) \left( -\frac{1}{\pi} \text{Im} \chi^{\mp\pm}(\omega - \omega') g_{0\sigma}(\omega') \right). \quad (48)$$

The equations (30) and (48) constitute a self-consistent system of equations for the single-particle Green function of SIAM. Note that spin-up and spin-down electrons are correlated when they occupy the impurity level. So, this really improves the standard mean-field theory in which just these correlations were missed. The role of electron-electron correlation becomes much more crucial for the case of strong correlation.

## 5 SIAM. Strong Correlation

The simplest relevant algebra of the operators used for the description of the strong correlation has a similar form as for that of the Hubbard model.<sup>28,32,79,81</sup> Let us represent the matrix Green function (27) in the following form

$$\hat{G}(\omega) = \sum_{\alpha\beta} \begin{pmatrix} \langle\langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle c_{k\sigma} | d_{0\beta\sigma}^\dagger \rangle\rangle \\ \langle\langle d_{0\alpha\sigma} | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle d_{0\alpha\sigma} | d_{0\beta\sigma}^\dagger \rangle\rangle \end{pmatrix}. \quad (49)$$

Here the operators  $d_{0\alpha\sigma}$  and  $d_{0\beta\sigma}^\dagger$  are

$$d_{i\alpha\sigma} = n_{i-\sigma}^\alpha a_{i\sigma}, (\alpha = \pm); \quad n_{i\sigma}^+ = n_{i\sigma}, \quad n_{i\sigma}^- = (1 - n_{i\sigma}); \\ \sum n_{i\sigma}^\alpha = 1; \quad n_{i\sigma}^\alpha n_{i\sigma}^\beta = \delta_{\alpha\beta} n_{i\sigma}^\alpha; \quad \sum_\alpha d_{i\alpha\sigma} = a_{i\sigma}. \quad (50)$$

The new operators  $d_{i\alpha\sigma}$  and  $d_{j\beta\sigma}^\dagger$  have complicated commutation rules, namely,

$$[d_{i\alpha\sigma}, d_{j\beta\sigma}^\dagger]_+ = \delta_{ij} \delta_{\alpha\beta} n_{i-\sigma}^\alpha. \quad (51)$$

Then we proceed by analogy with the calculations for the Hubbard model. The equation of motion for the auxiliary matrix Green function

$$\hat{F}_\sigma(\omega) = \begin{pmatrix} \langle\langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle c_{k\sigma} | d_{0+\sigma}^\dagger \rangle\rangle & \langle\langle c_{k\sigma} | d_{0-\sigma}^\dagger \rangle\rangle \\ \langle\langle d_{0+\sigma} | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle d_{0+\sigma} | d_{0+\sigma}^\dagger \rangle\rangle & \langle\langle d_{0+\sigma} | d_{0-\sigma}^\dagger \rangle\rangle \\ \langle\langle d_{0-\sigma} | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle d_{0-\sigma} | d_{0+\sigma}^\dagger \rangle\rangle & \langle\langle d_{0-\sigma} | d_{0-\sigma}^\dagger \rangle\rangle \end{pmatrix}$$

is of the following form

$$\hat{E} \hat{F}_\sigma(\omega) - \hat{I} = \hat{D}, \quad (52)$$

where the following matrix notation were used

$$\hat{E} = \begin{pmatrix} (\omega - \epsilon_k) & -V_k & -V_k \\ 0 & (\omega - E_{0\sigma} - U_+) & 0 \\ 0 & 0 & (\omega - E_{0\sigma} - U_-) \end{pmatrix}, \quad (53)$$

$$\hat{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & n_{0-\sigma}^+ & 0 \\ 0 & 0 & n_{0-\sigma}^- \end{pmatrix}, \quad U_\alpha = \begin{cases} U, & \alpha = + \\ 0, & \alpha = - \end{cases} \quad (54)$$

Here  $\hat{D}$  is a higher-order Green function, with the following structure<sup>7,11</sup>

$$\hat{D}(\omega) = \begin{pmatrix} 0 & 0 & 0 \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{pmatrix}. \quad (55)$$

In accordance with the general method of irreducible Green functions, we define the matrix irreducible Green function:

$$\hat{D}^{(ir)}(\omega) = \hat{D} - \sum_{\alpha} \begin{pmatrix} A^{+\alpha} \\ A^{-\alpha} \end{pmatrix} (G_{\sigma}^{\alpha+} \quad G_{\sigma}^{\alpha-}). \quad (56)$$

Here the notation were used:

$$A^{++} = \frac{\langle (f_{0-\sigma}^{\dagger} c_{p-\sigma} + c_{p-\sigma}^{\dagger} f_{0-\sigma})(n_{0\sigma} - n_{0-\sigma}) \rangle}{\langle n_{0-\sigma} \rangle}, \quad (57)$$

$$A^{--} = \frac{-\langle (f_{0-\sigma}^{\dagger} c_{p-\sigma} + c_{p-\sigma}^{\dagger} f_{0-\sigma})(1 + n_{0\sigma} - n_{0-\sigma}) \rangle}{\langle 1 - n_{0-\sigma} \rangle}, \quad (58)$$

$$A^{-+} = A^{++}, \quad A^{+-} = -A^{--}. \quad (59)$$

The generalized mean-field Green function is defined by

$$\hat{E}\hat{F}_{\sigma}^0(\omega) - \hat{I} = 0; \quad G^0 = \sum_{\alpha\beta} F_{\alpha\beta}^0. \quad (60)$$

From the last definition we find that

$$\begin{aligned} \langle \langle f_{0\sigma} | f_{0\sigma}^{\dagger} \rangle \rangle_{\omega}^0 &= \frac{\langle n_{0-\sigma} \rangle}{\omega - E_{0\sigma} - U_+ - \sum_p V_p A^{++}} \left( 1 + \frac{\sum_p V_p A^{-+}}{\omega - E_{0\sigma} - U_-} \right) \\ &+ \frac{1 - \langle n_{0-\sigma} \rangle}{\omega - E_{0\sigma} - U_- - \sum_p V_p A^{--}} \left( 1 + \frac{\sum_p V_p A^{+-}}{\omega - E_{0\sigma} - U_+} \right), \end{aligned} \quad (61)$$

$$\langle \langle c_{k\sigma} | c_{k\sigma}^{\dagger} \rangle \rangle_{\omega}^0 = (\omega - \epsilon_k - |V_k|^2 F^{at}(\omega))^{-1}, \quad (62)$$

where

$$F^{at} = \frac{\langle n_{0-\sigma} \rangle}{\omega - E_{0\sigma} - U_+} + \frac{1 - \langle n_{0-\sigma} \rangle}{\omega - E_{0\sigma} - U_-} \quad (63)$$

For  $V_p = 0$ , we obtain, from solution (61), the atomic solution  $F^{at}$ . The conduction electron Green function (62) also gives a correct expression for  $V_k = 0$ .

## 6 IGF Method and Interpolation Solution of SIAM

To show explicitly the flexibility of the IGF method, we consider a more extended new algebra of operators from which the relevant matrix Green function should be constructed to make the connection with the interpolation solution of the Anderson model.<sup>11</sup> Our approach was stimulated by the works by J. Hubbard.<sup>29,30,31</sup>

Let us consider the following equation of motion in the matrix form

$$\sum_p \hat{F}(p, k) \hat{G}_{p\sigma}(\omega) = \hat{I} + \sum_p V_p \hat{D}_p(\omega), \quad (64)$$

where  $\hat{G}$  is the initial  $4 \times 4$  matrix Green function and  $D$  is the higher-order Green function:

$$\hat{G}_\sigma = \begin{pmatrix} G_{11} & G_{12} & G_{13} & G_{14} \\ G_{21} & G_{22} & G_{23} & G_{24} \\ G_{31} & G_{32} & G_{33} & G_{34} \\ G_{41} & G_{42} & G_{43} & G_{44} \end{pmatrix}. \quad (65)$$

Here the following notation were used

$$\begin{aligned} G_{11} &= \langle\langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle; & G_{12} &= \langle\langle c_{k\sigma} | f_{0\sigma}^\dagger \rangle\rangle; \\ G_{13} &= \langle\langle c_{k\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle\rangle; & G_{14} &= \langle\langle c_{k\sigma} | c_{k\sigma}^\dagger n_{0-\sigma} \rangle\rangle; \\ G_{21} &= \langle\langle f_{0\sigma} | c_{k\sigma}^\dagger \rangle\rangle; & G_{22} &= \langle\langle f_{0\sigma} | f_{0\sigma}^\dagger \rangle\rangle; \\ G_{23} &= \langle\langle f_{0\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle\rangle; & G_{24} &= \langle\langle f_{0\sigma} | c_{k\sigma}^\dagger n_{0-\sigma} \rangle\rangle; \\ G_{31} &= \langle\langle f_{0\sigma} n_{0-\sigma} | c_{k\sigma}^\dagger \rangle\rangle; & G_{32} &= \langle\langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger \rangle\rangle; \\ G_{33} &= \langle\langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle\rangle; & G_{34} &= \langle\langle f_{0\sigma} n_{0-\sigma} | c_{k\sigma}^\dagger n_{0-\sigma} \rangle\rangle; \\ G_{41} &= \langle\langle c_{k\sigma} n_{0-\sigma} | c_{k\sigma}^\dagger \rangle\rangle; & G_{42} &= \langle\langle c_{k\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger \rangle\rangle; \\ G_{43} &= \langle\langle c_{k\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle\rangle; & G_{44} &= \langle\langle c_{k\sigma} n_{0-\sigma} | c_{k\sigma}^\dagger n_{0-\sigma} \rangle\rangle. \end{aligned} \quad (66)$$

We avoid to write down explicitly the relevant 16 Green functions, of which the matrix Green function  $D$  consist, for the brevity. For our aims, it is enough to proceed forth in the following way.

The equation (64) results from the first-time differentiation of the Green function  $G$  and is a starting point for the IGF approach. Let us introduce the irreducible part for the higher-order Green function  $D$  in the following way

$$\hat{D}_\beta^{(ir)} = \hat{D}_\beta - \sum_\alpha \hat{L}^{\beta\alpha} \hat{G}_{\alpha\beta}; \quad (\alpha, \beta) = (1, 2, 3, 4) \quad (67)$$

and define the generalized mean field Green function according to

$$\sum_p \hat{F}(p, k) \hat{G}_{p\sigma}^{MF}(\omega) = \hat{I}. \quad (68)$$

Then, we are able to write down explicitly the Dyson equation (23) and the exact expression for the self-energy  $M$  in the matrix form:

$$\hat{M}_{k\sigma}(\omega) = \hat{I}^{-1} \sum_{p,q} V_p V_q \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & M_{33} & M_{34} \\ 0 & 0 & M_{43} & M_{44} \end{pmatrix} \hat{I}^{-1}. \quad (69)$$

Here the matrix  $\hat{I}$  is given by

$$\hat{I} = \begin{pmatrix} 1 & 0 & 0 & \langle n_{0-\sigma} \rangle \\ 0 & 1 & \langle n_{0-\sigma} \rangle & 0 \\ 0 & \langle n_{0-\sigma} \rangle & \langle n_{0-\sigma} \rangle & 0 \\ \langle n_{0-\sigma} \rangle & 0 & 0 & \langle n_{0-\sigma} \rangle \end{pmatrix}, \quad (70)$$

and the matrix elements of  $M$  are of the form:

$$\begin{aligned} M_{33} &= (\langle\langle A_1^{(ir)}(p) | B_1^{(ir)}(q) \rangle\rangle)^{(p)}, & M_{34} &= (\langle\langle A_1^{(ir)}(p) | B_2^{(ir)}(k, q) \rangle\rangle)^{(p)} \\ M_{43} &= (\langle\langle A_2^{(ir)}(k, p) | B_1^{(ir)}(q) \rangle\rangle)^{(p)}, & M_{44} &= (\langle\langle A_2^{(ir)}(k, p) | B_2^{(ir)}(k, q) \rangle\rangle)^{(p)}. \end{aligned} \quad (71)$$

Here

$$\begin{aligned}
A_1(p) &= (c_{p-\sigma}^\dagger f_{0\sigma} f_{0-\sigma} - c_{p-\sigma} f_{0-\sigma}^\dagger f_{0\sigma}); \\
A_2(k, p) &= (c_{k\sigma} f_{0-\sigma}^\dagger c_{p-\sigma} - c_{k\sigma} c_{p-\sigma}^\dagger f_{0-\sigma}); \\
B_1(p) &= (f_{0\sigma}^\dagger c_{p-\sigma}^\dagger f_{0-\sigma} - f_{0\sigma}^\dagger f_{0-\sigma}^\dagger c_{p-\sigma}); \\
B_2(k, p) &= (c_{k\sigma}^\dagger c_{p-\sigma}^\dagger f_{0-\sigma} - c_{k\sigma}^\dagger f_{0-\sigma}^\dagger c_{p-\sigma}).
\end{aligned} \tag{72}$$

Since the self-energy  $M$  describes the processes of inelastic scattering of electrons ( $c - c$ ,  $f - f$ , and  $c - f$  types), its approximate representation would be defined by the nature of physical assumptions about this scattering.

To get an idea about the functional structure of our generalized mean field solution (68), let us write down the matrix element  $G_{33}^{MF}$ :

$$\begin{aligned}
G_{33}^{MF} &= \langle\langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle\rangle = \\
&= \frac{\langle n_{0-\sigma} \rangle}{\omega - \epsilon_f^{MF} - U - S^{MF}(\omega) - Y(\omega)} + \\
&= \frac{\langle n_{0-\sigma} \rangle Z(\omega)}{(\omega - \epsilon_f^{MF} - U - S^{MF}(\omega) - Y(\omega))(\omega - E_{0\sigma} - S(\omega))};
\end{aligned} \tag{73}$$

$$Y(\omega) = \frac{UZ(\omega)}{\omega - E_{0\sigma} - S(\omega)}; \tag{74}$$

$$Z(\omega) = S(\omega) \sum_p \frac{V_p L^{41}}{\omega - \epsilon_p^{MF}} + \sum_p \frac{|V_p|^2 L^{42}}{\omega - \epsilon_p^{MF}} + S(\omega) L^{31} + \sum_p V_p L^{32}. \tag{75}$$

Here the coefficients  $L^{41}$ ,  $L^{42}$ ,  $L^{31}$ , and  $L^{32}$  are certain complicated averages (see definition (67)) from which the functional of the generalized mean field is build. To clarify the functional structure of the obtained solution, let us consider our first equation of motion (64), before introducing the irreducible Green functions (67). Let us put in this equation the higher-order Green function  $D = 0$ . To distinguish this simplest equation from the generalized mean field one (68), we write it in the following form

$$\sum_p \hat{F}(p, k) \hat{G}^0(p, \omega) = \hat{I}. \tag{76}$$

The corresponding matrix elements which we are interested in here read

$$\begin{aligned}
G_{22}^0 &= \langle\langle f_{0\sigma} | f_{0\sigma}^\dagger \rangle\rangle = \\
&= \frac{1 - \langle n_{0-\sigma} \rangle}{\omega - E_{0\sigma} - S(\omega)} + \frac{\langle n_{0-\sigma} \rangle}{\omega - E_{0\sigma} - S(\omega) - U},
\end{aligned} \tag{77}$$

$$G_{33}^0 = \langle\langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle\rangle = \frac{\langle n_{0-\sigma} \rangle}{\omega - E_{0\sigma} - S(\omega) - U}, \tag{78}$$

$$G_{32}^0 = \langle\langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger \rangle\rangle = G_{33}^0. \tag{79}$$

The conclusion is rather evident. The simplest interpolation solution follows from our matrix Green function (65) in the lowest order in  $V$ , even before introduction of generalized mean field corrections, not speaking about the self-energy corrections. The two Green functions  $G_{32}^0$  and  $G_{33}^0$  are equal only in the lowest order in  $V$ . It is quite clear that our full solution (24) that includes the self-energy corrections is much more richer.

It is worthwhile to stress that our  $4 \times 4$  matrix generalized mean field Green function (65) gives only approximate description of suitable mean fields. If we consider more extended algebra of relevant operators, we get the more correct structure of the relevant generalized mean field.

## 7 Quasiparticle Dynamics of SIAM

To demonstrate more clearly the advantages of the irreducible Green functions method for SIAM, it is worthwhile to emphasize a few important points about the approach based on the equations-of-motion for the Green functions. To give a more instructive discussion, let us consider the single-particle Green function of localized electrons  $G_\sigma = \langle\langle f_{0\sigma}|f_{0\sigma}^\dagger \rangle\rangle$ . The simplest approximate "interpolation" solution of SIAM is of the form:

$$G_\sigma(\omega) = \frac{1}{\omega - E_{0\sigma} - S(\omega)} + \frac{U\langle n_{0-\sigma} \rangle}{(\omega - E_{0\sigma} - S(\omega) - U)(\omega - E_{0\sigma} - S(\omega))} = \frac{1 - \langle n_{0-\sigma} \rangle}{\omega - E_{0\sigma} - S(\omega)} + \frac{\langle n_{0-\sigma} \rangle}{\omega - E_{0\sigma} - S(\omega) - U}. \quad (80)$$

The values of  $n_\sigma$  are determined through the self-consistency equation

$$n_\sigma = \langle n_{0\sigma} \rangle = -\frac{1}{\pi} \int dE n(E) \text{Im} G_\sigma(E, n_\sigma). \quad (81)$$

The *atomic-like* interpolation solution (80) reproduces correctly the two limits:

$$G_\sigma(\omega) = \frac{1 - \langle n_{0-\sigma} \rangle}{\omega - E_{0\sigma}} + \frac{\langle n_{0-\sigma} \rangle}{\omega - E_{0\sigma} - U}, \quad \text{for } V = 0, \quad (82)$$

$$G_\sigma(\omega) = \frac{1}{\omega - E_{0\sigma} - S(\omega)}, \quad \text{for } U = 0, \quad (83)$$

where

$$S(\omega) = \sum_k \frac{|V_k|^2}{\omega - \epsilon_k}. \quad (84)$$

The important point about equations (82),(83) is that any approximate solution of SIAM should be consistent with it. Let us remind how to get solution (82). It follows from the system of equations for small- $V$  limit:

$$\begin{aligned} (\omega - E_{0\sigma} - S(\omega))\langle\langle f_{0\sigma}|f_{0\sigma}^\dagger \rangle\rangle_\omega &= 1 + U\langle\langle f_{0\sigma}n_{0-\sigma}|f_{0\sigma}^\dagger \rangle\rangle_\omega, \\ (\omega - E_{0\sigma} - U)\langle\langle f_{0\sigma}n_{0-\sigma}|f_{0\sigma}^\dagger \rangle\rangle_\omega &\approx \\ \langle n_{0-\sigma} \rangle + \sum_k V_k \langle\langle c_{k\sigma}n_{0\sigma}|f_{0\sigma}^\dagger \rangle\rangle_\omega, & \quad (85) \end{aligned}$$

$$(\omega - \epsilon_k)\langle\langle c_{k\sigma}n_{0-\sigma}|f_{0\sigma}^\dagger \rangle\rangle_\omega = V_k\langle\langle f_{0\sigma}n_{0-\sigma}|f_{0\sigma}^\dagger \rangle\rangle_\omega. \quad (86)$$

Note that the equations (85) and (86) are approximate; they include two more terms.

We now proceed further. The starting point is the system of equations:

$$(\omega - E_{0\sigma} - S(\omega))\langle\langle f_{0\sigma}|f_{0\sigma}^\dagger \rangle\rangle = 1 + U\langle\langle f_{0\sigma}n_{0-\sigma}|f_{0\sigma}^\dagger \rangle\rangle, \quad (87)$$

$$\begin{aligned} (\omega - E_{0\sigma} - U)\langle\langle f_{0\sigma}n_{0-\sigma}|f_{0\sigma}^\dagger \rangle\rangle &= \langle n_{0-\sigma} \rangle + \sum_k V_k \left( \langle\langle c_{k\sigma}n_{0-\sigma}|f_{0\sigma}^\dagger \rangle\rangle - \right. \\ &\quad \left. \langle\langle c_{k-\sigma}f_{0-\sigma}^\dagger f_{0\sigma}|f_{0\sigma}^\dagger \rangle\rangle + \langle\langle c_{k-\sigma}^\dagger f_{0\sigma} f_{0-\sigma}|f_{0\sigma}^\dagger \rangle\rangle \right). \quad (88) \end{aligned}$$

Using a relatively simple decoupling procedure for a higher-order equation of motion, a qualitatively correct low-temperature spectral intensity can be calculated. The final expression for  $G$  for finite  $U$  is of the form

$$\langle\langle f_{0\sigma}|f_{0\sigma}^\dagger \rangle\rangle = \frac{1}{\omega - E_{0\sigma} - S(\omega) + US_1(\omega)} + \frac{U\langle n_{0-\sigma} \rangle + UF_1(\omega)}{K(\omega)(\omega - E_{0\sigma} - S(\omega) + US_1(\omega))}, \quad (89)$$

where  $F_1$ ,  $S_1$ , and  $K$  are certain complicated expressions. We write down explicitly the infinite  $U$  approximate Green function:

$$\langle\langle f_{0\sigma}|f_{0\sigma}^\dagger\rangle\rangle \cong \frac{1 - \langle n_{0-\sigma}\rangle - F_\sigma(\omega)}{\omega - E_{0\sigma} - S(\omega) - Z_\sigma^1(\omega)}. \quad (90)$$

The following notation were used:

$$F_\sigma = V \sum_k \frac{\langle f_{0-\sigma}^\dagger c_{k-\sigma} \rangle}{\omega - \epsilon_k}, \quad (91)$$

$$Z_\sigma^1 = V^2 \sum_{q,k} \frac{\langle c_{q-\sigma}^\dagger c_{k-\sigma} \rangle}{\omega - \epsilon_k} - S(\omega) V \sum_k \frac{\langle f_{0-\sigma}^\dagger c_{k-\sigma} \rangle}{\omega - \epsilon_k}. \quad (92)$$

We putted here  $V_k \simeq V$  for brevity. The functional structure of the single-particle Green function (89) is quite transparent. The expression in the numerator of (89) plays the role of an effective *dynamical mean field*, proportional to  $\langle f_{0-\sigma}^\dagger c_{k-\sigma} \rangle$ . In the denominator, instead of bare shift  $S(\omega)$  (34) we have an *effective shift*  $S^1 = S(\omega) + Z_\sigma^1(\omega)$ . The choice of the specific procedure of decoupling for the higher-order equation of motion specifies the selected *generalized mean fields* and *effective shifts*.

## 8 Complex Expansion for a Propagator

We now proceed with analytic many-body consideration. One can attempt to consider a suitable solution for the SIAM starting from the following exact relation derived in paper:<sup>11</sup>

$$\langle\langle f_{0\sigma}|f_{0\sigma}^\dagger\rangle\rangle = g^0 + g^0 P g^0, \quad (93)$$

$$g^0 = (\omega - E_{0\sigma} - S(\omega))^{-1}, \quad (94)$$

$$P = U \langle n_{0-\sigma} \rangle + U^2 \langle\langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle\rangle. \quad (95)$$

The advantage of the equation (93) is that it is a pure **identity** and does not includes any approximation. If we insert our generalized mean field solution (90) into (93), we get an essentially new dynamic solution of SIAM constructed on the basis of the complex (combined) expansion of the propagator in both  $U$  and  $V$  parameters and reproducing exact solutions of SIAM for  $V = 0$  and  $U = 0$ . It generalizes (even on the mean-field level) the known approximate solutions of the Anderson model.

Having emphasized the importance of the role of equation (93), let us see now what is the best possible fit for higher-order Green function in (95). We consider the equation of motion for it:

$$\begin{aligned} (\omega - E_{0\sigma} - U) \langle\langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle\rangle &= \langle n_{0-\sigma} \rangle + \\ &\sum_k V_k \langle\langle c_{k\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle\rangle + \\ \langle\langle c_{k-\sigma}^\dagger f_{0\sigma} f_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle\rangle &- \langle\langle c_{k-\sigma} f_{0-\sigma} f_{0\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle\rangle. \end{aligned} \quad (96)$$

We may think of it as defining new kinds of elastic and inelastic scattering processes that contribute to the formation of generalized mean fields and self-energy (damping) corrections. The construction of suitable mean fields can be quite nontrivial, and to describe these contributions self-consistently, let us consider the equations of motion for higher-order Green functions in the



r.h.s. of (96)

$$\begin{aligned}
& (\omega - \epsilon_k) \langle \langle c_{k\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle = \\
& \quad V \langle \langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle + \\
& \sum_p V (\langle \langle c_{k\sigma} f_{0-\sigma}^\dagger c_{p-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle - \langle \langle c_{k\sigma} c_{p-\sigma}^\dagger f_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle),
\end{aligned} \tag{97}$$

$$\begin{aligned}
& (\omega - \epsilon_k - E_{0\sigma} + E_{0-\sigma}) \langle \langle c_{k-\sigma} f_{0-\sigma}^\dagger f_{0\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle \\
& \quad = - \langle f_{0-\sigma}^\dagger c_{k-\sigma} n_{0\sigma} \rangle - \\
& \quad \quad V \langle \langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle + \\
& \sum_p V (\langle \langle c_{k-\sigma} f_{0-\sigma}^\dagger c_{p\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle - \langle \langle c_{k-\sigma} c_{p-\sigma}^\dagger f_{0\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle),
\end{aligned} \tag{98}$$

$$\begin{aligned}
& (\omega + \epsilon_k - E_{0\sigma} - E_{0-\sigma} - U) \langle \langle c_{k-\sigma}^\dagger f_{0\sigma} f_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle \\
& \quad = - \langle c_{k-\sigma}^\dagger f_{0\sigma} f_{0\sigma}^\dagger f_{0-\sigma} \rangle + \\
& \quad \quad V \langle \langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle + \\
& \sum_p V (\langle \langle c_{k-\sigma}^\dagger c_{p\sigma} f_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle + \langle \langle c_{k-\sigma}^\dagger f_{0\sigma} c_{p-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle).
\end{aligned} \tag{99}$$

Now let us see how to proceed further to get a suitable functional structure of the relevant solution. The intrinsic nature of the system of the equations of motion (97) - (99) suggests to consider the following approximations:

$$(\omega - \epsilon_k) \langle \langle c_{k\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle \approx V \langle \langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle, \tag{100}$$

$$\begin{aligned}
& (\omega - \epsilon_k - E_{0\sigma} + E_{0-\sigma}) \langle \langle c_{k-\sigma} f_{0-\sigma}^\dagger f_{0\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle \approx - \langle f_{0-\sigma}^\dagger c_{k-\sigma} n_{0\sigma} \rangle \\
& \quad - V (\langle \langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle - \langle \langle c_{k-\sigma} c_{k-\sigma}^\dagger f_{0\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle),
\end{aligned} \tag{101}$$

$$\begin{aligned}
& (\omega + \epsilon_k - E_{0\sigma} - E_{0-\sigma} - U) \langle \langle c_{k-\sigma}^\dagger f_{0\sigma} f_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle \approx - \langle c_{k-\sigma}^\dagger f_{0\sigma} f_{0\sigma}^\dagger f_{0-\sigma} \rangle + \\
& \quad V (\langle \langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle + \langle \langle c_{k-\sigma}^\dagger f_{0\sigma} c_{k-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle).
\end{aligned} \tag{102}$$

It is transparent that the construction of approximations (100) - (102) is related with the small- $V$  expansion and is not unique, but very natural. As a result, we find the explicit expression for Green function in (95)

$$\langle \langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle \approx \frac{\langle n_{0-\sigma} \rangle - F_\sigma^1(\omega)}{\omega - E_{0\sigma} - U - S_1(\omega)}. \tag{103}$$

Here the following notation were used:

$$S_1(\omega) = S(\omega) \tag{104}$$

$$+ \sum_k |V|^2 \left( \frac{1}{\omega - \epsilon_k - E_{0\sigma} + E_{0-\sigma}} + \frac{1}{\omega + \epsilon_k - E_{0\sigma} - E_{0-\sigma} - U} \right),$$

$$F_\sigma^1 = \sum_k (V F_2 + V^2 F_3), \tag{105}$$

$$F_2 = \frac{\langle c_{k-\sigma}^\dagger f_{0\sigma} f_{0\sigma}^\dagger f_{0-\sigma} \rangle}{\omega + \epsilon_k - E_{0\sigma} - E_{0-\sigma} - U} + \frac{\langle f_{0-\sigma}^\dagger c_{k-\sigma} n_{0\sigma} \rangle}{\omega - \epsilon_k - E_{0\sigma} + E_{0-\sigma}}, \tag{106}$$

$$F_3 = \frac{\langle \langle c_{k-\sigma} c_{k-\sigma}^\dagger f_{0\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle}{\omega - \epsilon_k - E_{0\sigma} + E_{0-\sigma}} + \frac{\langle \langle c_{k-\sigma}^\dagger f_{0\sigma} c_{k-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle \rangle}{\omega + \epsilon_k - E_{0\sigma} - E_{0-\sigma} - U}. \tag{107}$$

Now one can substitute the Green function in (95) by the expression (103). This gives a new approximate dynamic solution of SIAM where the complex expansion both in  $U$  and  $V$  was incorporated. The important observation is that this new solution satisfies both the limits (82). For example, if we wish to get a lowest order approximation up to  $U^2$  and  $V^2$ , it is very easy to notice that for  $V = 0$ :

$$\langle\langle f_{0\sigma} c_{k-\sigma}^\dagger c_{k-\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle\rangle \approx \frac{\langle c_{k-\sigma}^\dagger c_{k-\sigma} \rangle \langle n_{0-\sigma} \rangle}{\omega - E_{0\sigma} - U}, \quad (108)$$

$$\langle\langle c_{k-\sigma} c_{k-\sigma}^\dagger f_{0\sigma} | f_{0\sigma}^\dagger n_{0-\sigma} \rangle\rangle \approx \frac{\langle c_{k-\sigma} c_{k-\sigma}^\dagger \rangle \langle n_{0-\sigma} \rangle}{\omega - E_{0\sigma} - U}. \quad (109)$$

This results in the possibility to find explicitly all necessary quantities and, thus, to solve the problem in a self-consistent way. The main results of our IGF study is the exact Dyson equation for the full matrix Green function and a new derivation of the *generalized mean field* Green functions. The approximate explicit calculations of inelastic self-energy corrections are quite straightforward but tedious and too extended for their description. Here we want to emphasize an essentially new point of view on the derivation of the generalized mean fields for SIAM when we are interested in the interpolation finite temperature solution for the single-particle propagator. Our final solutions have the correct functional structure and differ essentially from previous solutions.

In summary, we presented here a consistent many-body approach to analytic dynamic solution of SIAM at finite temperatures and for a broad interval of the values of the model parameters. We used the exact result (93) to connect the single-particle Green function with higher-order Green function to obtain a complex combined expansion in terms of  $U$  and  $V$  for the propagator. We reformulated also the problem of searches for an appropriate many-body dynamic solution for SIAM in a way that provides us with an effective and workable scheme for constructing of advanced analytic approximate solutions for the single-particle Green functions on the level of the higher-order Green functions in a rather systematic self-consistent way. This procedure has the advantage that it systematically uses the principle of interpolation solution within the equation-of-motion approach for Green functions. The leading principle, which we used here was to look more carefully for the intrinsic functional structure of the required relevant solution and then to formulate approximations for the higher-order Green functions in accordance with this structure. Of course, there are important criteria to be met (mainly numerically), such as the question left open, whether the present approximation satisfies the Friedel sum rule (this question was left open in many other approximate solutions). A quantitative numerical comparison of self-consistent results e.g. the width and shape of the Kondo resonance in the near-integer regime of the SIAM would be crucial too. In the present consideration, we concentrated on the problem of correct functional structure of the single-particle Green function itself.

## 9 The Improved Interpolative Treatment of SIAM

For better understanding of the correct functional structure of the single-particle Green function the development of improved and reliable approximation schemes is still justified and necessary, and an effective interpolating approximations are desirable. The present section is devoted to the development of an improved interpolating approximation<sup>10,11</sup> for the dynamical properties of the SIAM. We will show that a self-consistent approximation can be formulated which reproduces all relevant exactly solvable limits of the model and interpolates between the strong- and the weak-coupling limit. This approach is complementary to the one described above.

We start by considering the equations of motion for the Fourier transformed Green function,

$$G_\sigma(\omega) = \langle\langle f_\sigma | f_\sigma^\dagger \rangle\rangle_\omega = -i \int_0^\infty dt \exp(i\omega t) \langle [f_{0\sigma}(t), f_{0\sigma}^\dagger]_+ \rangle : \quad (110)$$

$$(\omega - E_\sigma - S(\omega))\langle\langle f_\sigma | f_\sigma^\dagger \rangle\rangle_\omega = 1 + U\langle\langle f_\sigma n_{-\sigma} | f_\sigma^\dagger \rangle\rangle_\omega = 1 + \Sigma_\sigma(\omega)\langle\langle f_\sigma | f_\sigma^\dagger \rangle\rangle_\omega. \quad (111)$$

Here the quantity  $\Sigma_\sigma(\omega)$  may be conditionally interpreted as the one-particle self-energy and

$$S(\omega) = \sum_k \frac{|V|^2}{\omega - \epsilon_k}. \quad (112)$$

We want to develop an *interpolating* solution for the SIAM, i.e. a solution which is applicable in both, the weak-coupling limit (and thus the exactly solvable band limit) and the strong-coupling limit (and thus the atomic limit). As it was shown earlier, the simplest approximative *interpolating* solution has the form:

$$G_\sigma(\omega) = \frac{1 - \langle n_{-\sigma} \rangle}{\omega - E_\sigma - S(\omega)} + \frac{\langle n_{-\sigma} \rangle}{\omega - E_\sigma - S(\omega) - U}. \quad (113)$$

Here  $\langle n_{-\sigma} \rangle$  denotes the occupation number of  $f$ -electrons with spin  $\sigma$ . This is just the analogue of the *Hubbard III* approximation<sup>28</sup> for the SIAM. As for the Hubbard model, however, Fermi liquid properties and the Friedel sum rule, which hold for the SIAM at least order by order within the  $U$ -perturbation theory, are violated within this simple approximation.

An approximation, which automatically fulfills Fermi liquid properties and sum rules, is provided by the self-consistent second order  $U$ -perturbation treatment (SOPT) and is given by:

$$\Sigma_\sigma(i\omega_n) = U\langle n_{-\sigma} \rangle - \left(\frac{U}{\beta}\right)^2 \sum_{\omega_1, \nu} G_\sigma(i\omega_n + i\nu)G_{-\sigma}(i\omega_1 - i\nu)G_{-\sigma}(i\omega_1). \quad (114)$$

Here  $\omega_1(\nu)$  denote odd (even) Matsubara frequencies and  $\beta = 1/k_B T$ . One of our goals is to find some way to incorporate this SOPT into an interpolating dynamical solution of the SIAM. This means that the approximation for the self-energy shall be correct up to order  $U^2$  perturbationally around the band limit  $U = 0$  and also the atomic limit  $V = 0$  shall be fulfilled. This is the case for the SOPT around the Hartree-Fock solution, but only for the symmetric SIAM. For the general situation (position of the Fermi level relative to  $E_\sigma$  and  $E_\sigma + U$ ) a heuristic semi-empirical approach only for constructing such an approximation has been discussed in literature. Here our intention is to take into account the self-consistent-SOPT. Furthermore, the approximation shall not only fulfill the atomic limit  $V = 0$ , but it shall be correct up to order  $V^2$  in a strong-coupling expansion around the atomic limit.

The self-consistent inclusion of contributions in second (and fourth) order perturbation theory around the atomic limit is, in particular, important to properly account for the Kondo effect within the SIAM (Kondo temperature scale) and to reproduce the correct antiferromagnetic behavior in the strong-coupling limit of the Hubbard model. Especially the calculation of some magnetic properties for the Hubbard model and the well known Kondo effect for the SIAM shows the importance of second (and fourth) order perturbation theory around the atomic limit.

It was already mentioned that during the last decades several different refined many-body techniques have been applied to the SIAM, and many of these approaches are strong-coupling treatments around the atomic limit and can be classified as being correct up to a certain power in the hybridization  $V$ . When applied to the calculation of static properties many of these treatments, give reasonable results. But for the many-body dynamics the results of most of these approximations are not fully satisfactory, in particular as Fermi liquid properties and sum rules are violated. Furthermore, when applied to the finite- $U$  SIAM none of these approximation schemes reproduce the SOPT, i.e. these approaches are not correct in the weak-coupling limit up to order  $U^2$ .

To construct the interpolating approximation<sup>7,10,11,8</sup> for the SIAM fulfilling all desired properties mentioned above we start from the equation of motion for the higher order Green function

$\langle\langle f_\sigma n_{-\sigma} | f_\sigma^\dagger \rangle\rangle_\omega$ :

$$(\omega - E_\sigma - S(\omega) - U) \langle\langle f_\sigma n_{-\sigma} | f_\sigma^\dagger \rangle\rangle_\omega = \langle n_{-\sigma} \rangle - U \langle\langle f_\sigma f_{-\sigma} f_{-\sigma}^\dagger | f_\sigma^\dagger n_{-\sigma} \rangle\rangle_\omega.$$

With

$$[G_\sigma^{(0)}(\omega)]^{-1} = \omega - E_\sigma - S(\omega) \quad (115)$$

and the self-consistent summation

$$[G_\sigma^{(0)}(\omega)]^{-1} G_\sigma(\omega) = 1 + \Sigma_\sigma(\omega) G_\sigma(\omega), \quad (116)$$

we derive from this equations of motion the following exact relation

$$\Sigma_\sigma(\omega) = \frac{U \langle n_{-\sigma} \rangle + U^2 \mathcal{Z}(\omega) \frac{G_\sigma(\omega)}{1 + \Sigma_\sigma(\omega) G_\sigma(\omega)}}{1 - (U - \Sigma_\sigma(\omega)) G_\sigma(\omega)}. \quad (117)$$

Here the definition

$$\langle\langle f_\sigma f_{-\sigma} f_{-\sigma}^\dagger | f_\sigma^\dagger n_{-\sigma} \rangle\rangle_\omega = -\mathcal{Z}(\omega) \frac{G_\sigma(\omega)}{1 + \Sigma_\sigma(\omega) G_\sigma(\omega)} \quad (118)$$

was introduced.

Applying the equations of motion to the higher-order Green function

$$\langle\langle f_\sigma f_{-\sigma} f_{-\sigma}^\dagger | f_\sigma^\dagger n_{-\sigma} \rangle\rangle_\omega, \quad (119)$$

one obtains for the function  $\mathcal{Z}(z)$  the exact equation

$$\mathcal{Z}(\omega) = V \sum_{\mathbf{k}} \left\{ G_{1\sigma}(\mathbf{k}) - G_{2\sigma}(\mathbf{k}) + \frac{V}{\omega - \epsilon_{\mathbf{k}}} [G_{3\sigma}(\mathbf{k}) - G_{4\sigma}(\mathbf{k})] \right\}, \quad (120)$$

with  $\underline{\mathbf{k}} = (\mathbf{k}, \omega)$  and

$$G_{1\sigma}(\underline{\mathbf{k}}) = \langle\langle f_\sigma f_{-\sigma}^\dagger c_{\mathbf{k}-\sigma} | f_\sigma^\dagger n_{-\sigma} \rangle\rangle_\omega, \quad (121)$$

$$G_{2\sigma}(\underline{\mathbf{k}}) = \langle\langle f_\sigma c_{\mathbf{k}-\sigma}^\dagger f_{-\sigma} | f_\sigma^\dagger n_{-\sigma} \rangle\rangle_\omega, \quad (122)$$

$$G_{3\sigma}(\underline{\mathbf{k}}) = \sum_{\mathbf{q}} \langle\langle c_{\mathbf{k}\sigma} f_{-\sigma} c_{\mathbf{q}-\sigma}^\dagger | f_\sigma^\dagger n_{-\sigma} \rangle\rangle_\omega, \quad (123)$$

$$G_{4\sigma}(\underline{\mathbf{k}}) = \sum_{\mathbf{q}} \langle\langle c_{\mathbf{k}\sigma} c_{\mathbf{q}-\sigma} f_{-\sigma}^\dagger | f_\sigma^\dagger n_{-\sigma} \rangle\rangle_\omega. \quad (124)$$

Self-consistency in the perturbation theory defines the Green function:

$$[G_\sigma^{(0)}(\omega)]^{-1} G_\sigma(\omega) = 1 + \Sigma_\sigma(\omega) G_\sigma(\omega), \quad (125)$$

and leads to an infinite order resummation resulting in a self-consistent approximation.

In general, there are several possibilities to incorporate self-consistency, but most of these possibilities lead once more to an approximation being exact up to order  $V^2$  but not reproducing the weak-coupling limit. To be exact up to order  $V^2$  it is justified to replace the higher order Green functions on the right hand side of Eq. (120) by their lowest order contributions, which are given by

$$\begin{aligned} G_{1\sigma}(\underline{\mathbf{k}}) &= \frac{V}{\epsilon_{\mathbf{k}} - E_{-\sigma} - U} \left[ \frac{\langle n_{-\sigma} \rangle [f_{\mathbf{k}} - f(E_{-\sigma} + U)] + \langle n_{-\sigma} \rangle [1 - f_{\mathbf{k}}]}{\omega - \epsilon_{\mathbf{k}} - E_\sigma + E_{-\sigma}} - \frac{\langle n_{-\sigma} \rangle [1 - f_{\mathbf{k}}]}{\omega - E_\sigma - U} \right] + O(V^3), \\ G_{2\sigma}(\underline{\mathbf{k}}) &= \frac{V}{\epsilon_{\mathbf{k}} - E_{-\sigma}} \left[ \frac{(1 - \langle n_{-\sigma} \rangle) [f_{\mathbf{k}} - f(E_{-\sigma})] + [1 - f_{\mathbf{k}}] \langle n_{-\sigma} \rangle}{\omega + \epsilon_{\mathbf{k}} - E_\sigma - E_{-\sigma} - U} - \frac{\langle n_{-\sigma} \rangle [1 - f_{\mathbf{k}}]}{\omega - E_\sigma - U} \right] + O(V^3), \\ G_{3\sigma}(\underline{\mathbf{k}}) &= O(V^2), \quad G_{4\sigma}(\underline{\mathbf{k}}) = O(V^2), \end{aligned} \quad (126)$$

leading to a finite order  $V^2$  perturbation expansion of the self-energy (117). Here  $f(E) = \{\exp[(E - \mu)/k_B T] + 1\}^{-1}$  is the Fermi function,  $\mu$  the chemical potential and  $f_{\mathbf{k}} = f(\epsilon_{\mathbf{k}})$ .

For the higher order Green functions  $G_{i\sigma}(\mathbf{k})$  ( $i = 1, \dots, 4$ ) one can find an approximation which reproduces the exact relations (126) in lowest order in  $V$  and is simultaneously exact in lowest order in  $U$  (when Wick's theorem is applicable). One possibility for such an approximation is given by:

$$G_{1\sigma}(\mathbf{k}) = \frac{-\beta^{-2}}{\langle n_{-\sigma} \rangle \langle n_{\sigma} n_{-\sigma} \rangle} \sum_{\omega_1, \nu} \langle \langle f_{\sigma} | n_{-\sigma} f_{\sigma}^{\dagger} \rangle \rangle_{i\omega_n + i\nu} \langle \langle c_{\mathbf{k}-\sigma} | n_{\sigma} f_{-\sigma}^{\dagger} \rangle \rangle_{i\omega_1 - i\nu} \\ \times \langle \langle f_{-\sigma} n_{\sigma} | f_{-\sigma}^{\dagger} \rangle \rangle_{i\omega_1} + \frac{\langle f_{-\sigma}^{\dagger} c_{\mathbf{k}-\sigma} n_{\sigma} \rangle}{\langle n_{-\sigma} \rangle} \langle \langle f_{\sigma} n_{-\sigma} | f_{\sigma}^{\dagger} \rangle \rangle_{i\omega_n} \quad (127)$$

$$G_{2\sigma}(\mathbf{k}) = \frac{-\beta^{-2}}{(1 - \langle n_{-\sigma} \rangle) \langle n_{\sigma} n_{-\sigma} \rangle} \sum_{\omega_1, \nu} \left( \frac{\langle n_{-\sigma} \rangle}{\langle n_{-\sigma} \rangle - \langle n_{\sigma} n_{-\sigma} \rangle} \langle \langle f_{\sigma} | f_{-\sigma} f_{-\sigma}^{\dagger} f_{\sigma}^{\dagger} \rangle \rangle_{i\omega_n + i\nu} \right. \\ \times \langle \langle f_{-\sigma} | n_{\sigma} f_{-\sigma}^{\dagger} \rangle \rangle_{i\omega_1 - i\nu} - \langle \langle f_{\sigma} | n_{-\sigma} f_{\sigma}^{\dagger} \rangle \rangle_{i\omega_n + i\nu} \langle \langle f_{-\sigma} | f_{\sigma} f_{\sigma}^{\dagger} f_{-\sigma}^{\dagger} \rangle \rangle_{i\omega_1 - i\nu} \left. \right) \\ \times \langle \langle f_{-\sigma} f_{\sigma} f_{\sigma}^{\dagger} | c_{\mathbf{k}-\sigma}^{\dagger} \rangle \rangle_{i\omega_1} + \frac{\langle f_{\sigma} f_{\sigma}^{\dagger} c_{\mathbf{k}-\sigma}^{\dagger} f_{-\sigma} \rangle}{1 - \langle n_{-\sigma} \rangle} \langle \langle f_{\sigma} n_{-\sigma} | f_{\sigma}^{\dagger} \rangle \rangle_{i\omega_n} \quad (128)$$

and the Green function  $G_{3\sigma}, G_{4\sigma}$  are decoupled according to the theorem of Wick. Since the approximation does not violate the theorem of Wick for small  $U$ , it automatically satisfies the SOPT, i.e., expanding Eq. (117) for small  $U$  up to second order in  $U$  leads to the SOPT for the self-energy. Also the  $V^2$ -limit is not violated since the Green function  $G_{3\sigma}, G_{4\sigma}$  are themselves proportional to  $V^2$ , leading in Eq. (120) to  $V^4$  terms. Therefore, our approximation leads to an expression for the self-energy of the SIAM, which is exact at least up to order  $U^2$  in a weak coupling expansion and up to order  $V^2$  in a strong coupling expansion. The structure of the chosen approximation (127) and (128) and of the decoupling for the Green function  $G_{3\sigma}, G_{4\sigma}$  according to the theorem of Wick has a similar analytical structure as the SOPT, (which can be calculated numerically very fast and accurate). Hence the explicit numerical calculations within this treatment are of the same order of complexity as those of the self-consistent-SOPT calculations.

Notice that in principle it is possible to systematically improve the above approximation. Since the self-consistent summation (117), (120) is formally exact, the next step would be the similar construction of an approximation for the Green functions  $G_{3\sigma}, G_{4\sigma}$  (and for Green functions of a similar structure occurring in a further application of the equations of motion to the Green functions  $G_{1\sigma}, G_{2\sigma}$ ) being exact in order  $V^2$  and simultaneously satisfying the theorem of Wick; as the Green functions  $G_{3\sigma}$  etc. have already a prefactor  $V^2$  in (120) this leads to an approximation for  $\mathcal{S}$  and thus the self-energy  $\Sigma_{\sigma}(\omega)$  being exact up to order  $V^4$  in the strong-coupling limit and simultaneously in order  $U^2$  in the weak-coupling limit. Furthermore, already from the structure of the exact equation (117) it is clear that our new approximation can be considered as a systematic improvement of the *Hubbard-III* approximation (113), which is known to be reasonable concerning the high-frequency behavior of the dynamical quantities and concerning the reproduction of the metal-insulator transition in the Hubbard model.

The improved approach goes beyond the *Hubbard-III* approximation<sup>28</sup> including all self-energy contributions in order  $U^2$  and thus reproducing the SOPT. This is important to fulfill the Fermi liquid properties at least for small  $U$ , and in this respect the approach should be as good as the related attempts.

On the other hand, the new approach is also exact up to order  $V^2$  and is, therefore, as good as standard equations of motion decoupling procedures are, which qualitatively describe important items like Kondo peak, Kondo temperature scale, etc.

When interpreting these standard equations of motion decouplings as generalized mean-field treatments, because the decoupling consists in a replacement of a higher order Green function by a product of an expectation value with a lower order Green function, our new approximation can be considered to be a kind of dynamical mean-field approximation, because the approximation (127), (128) consists in the replacement of a higher order Green function by combinations of products of (time-dependent) lower order Green functions.

Finally the approach is not a completely uncontrolled approximation, as it is exact up to certain orders ( $V^2$ ,  $U^2$ ) of systematic perturbation theory. It is, however, as any self-consistent approximate treatment is, uncontrolled in the way it takes into account infinite order resummations of arbitrary order in  $U$  and  $V$  by the self-consistent requirement, which is unavoidable to reproduce both limits.

In summary, an improved interpolating approximation for the SIAM has been developed, which recovers the exactly solvable limits  $V = 0$  and  $U = 0$  and which is even more at least correct up to order  $V^2$  in a strong-coupling expansion and simultaneously up to order  $U^2$  in a weak-coupling expansion.

## 10 Quasiparticle Many-Body Dynamics of PAM

The main drawback of the Hartree-Fock type solution of PAM (6) is that it ignores the correlations of the "up" and "down" electrons. In this section, we will take into account the latter correlations in a self-consistent way using the IGF method. We consider the relevant matrix Green function of the form (cf. (27))

$$\hat{G}(\omega) = \begin{pmatrix} \langle\langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle c_{k\sigma} | f_{k\sigma}^\dagger \rangle\rangle \\ \langle\langle f_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle f_{k\sigma} | f_{k\sigma}^\dagger \rangle\rangle \end{pmatrix}. \quad (129)$$

The equation of motion for Green function (129) reads

$$\begin{pmatrix} (\omega - \epsilon_k) & -V_k \\ -V_k & (\omega - E_k) \end{pmatrix} \begin{pmatrix} \langle\langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle c_{k\sigma} | f_{k\sigma}^\dagger \rangle\rangle \\ \langle\langle f_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle f_{k\sigma} | f_{k\sigma}^\dagger \rangle\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ +UN^{-1} \sum_{pq} \langle\langle A | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle A | f_{k\sigma}^\dagger \rangle\rangle \end{pmatrix}, \quad (130)$$

where  $A = f_{k+p\sigma} f_{p+q-\sigma}^\dagger f_{q-\sigma}$ . According to IGF method the definition of the irreducible parts in the equation of motion (130) are given by

$${}^{(ir)} \langle\langle f_{k+p\sigma} f_{p+q-\sigma}^\dagger f_{q-\sigma} | c_{k\sigma}^\dagger \rangle\rangle = \langle\langle f_{k+p\sigma} f_{p+q-\sigma}^\dagger f_{q-\sigma} | c_{k\sigma}^\dagger \rangle\rangle - \delta_{p,0} \langle n_{q-\sigma} \rangle \langle\langle f_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle, \quad (131)$$

$${}^{(ir)} \langle\langle f_{k+p\sigma} f_{p+q-\sigma}^\dagger f_{q-\sigma} | f_{k\sigma}^\dagger \rangle\rangle = \langle\langle f_{k+p\sigma} f_{p+q-\sigma}^\dagger f_{q-\sigma} | f_{k\sigma}^\dagger \rangle\rangle - \delta_{p,0} \langle n_{q-\sigma} \rangle \langle\langle f_{k\sigma} | f_{k\sigma}^\dagger \rangle\rangle. \quad (132)$$

After substituting these definitions into equation (130), we obtain

$$\begin{pmatrix} (\omega - \epsilon_k) & -V_k \\ -V_k & (\omega - E_\sigma(k)) \end{pmatrix} \begin{pmatrix} \langle\langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle c_{k\sigma} | f_{k\sigma}^\dagger \rangle\rangle \\ \langle\langle f_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle f_{k\sigma} | f_{k\sigma}^\dagger \rangle\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + UN^{-1} \sum_{pq} \begin{pmatrix} 0 & 0 \\ {}^{(ir)} \langle\langle A | c_{k\sigma}^\dagger \rangle\rangle & {}^{(ir)} \langle\langle A | f_{k\sigma}^\dagger \rangle\rangle \end{pmatrix}. \quad (133)$$

In the the following the notation will be used for brevity

$$E_\sigma(k) = E_k - Un_{-\sigma}; \quad n_{-\sigma} = \langle f_{k-\sigma}^\dagger f_{k-\sigma} \rangle. \quad (134)$$

The definition of the generalized mean field Green function (which, for the weak Coulomb correlation  $U$ , coincides with the Hartree-Fock mean field ) is evident. All inelastic renormalization terms are now related to the last term in the equation of motion (133). All elastic scattering ( or mean field) renormalization terms are included into the following mean-field Green function

$$\begin{pmatrix} (\omega - \epsilon_k) & -V_k \\ -V_k & (\omega - E_\sigma(k)) \end{pmatrix} \begin{pmatrix} \langle\langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle^0 & \langle\langle c_{k\sigma} | f_{k\sigma}^\dagger \rangle\rangle^0 \\ \langle\langle f_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle^0 & \langle\langle f_{k\sigma} | f_{k\sigma}^\dagger \rangle\rangle^0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

It is easy to find that (cf. (32) and (33))

$$\langle\langle f_{k\sigma} | f_{k\sigma}^\dagger \rangle\rangle^0 = \left( \omega - E_\sigma(k) - \frac{|V_k|^2}{\omega - \epsilon_k} \right)^{-1}, \quad (135)$$

$$\langle\langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle^0 = \left( \omega - \epsilon_k - \frac{|V_k|^2}{\omega - E_\sigma(k)} \right)^{-1}. \quad (136)$$

At this point, it is worthwhile to emphasize a significant difference between both the models, PAM and SIAM. The corresponding SIAM equation for generalized mean field Green function (31) reads

$$\sum_p \begin{pmatrix} (\omega - \epsilon_p) \delta_{pk} & -V_p \delta_{pk} \\ -V_p & \frac{1}{N} (\omega - E_{0\sigma} - U n_{-\sigma}) \end{pmatrix} \begin{pmatrix} \langle\langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle^0 & \langle\langle c_{k\sigma} | f_{0\sigma}^\dagger \rangle\rangle^0 \\ \langle\langle f_{0\sigma} | c_{k\sigma}^\dagger \rangle\rangle^0 & \langle\langle f_{0\sigma} | f_{0\sigma}^\dagger \rangle\rangle^0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (137)$$

This matrix notation for SIAM shows a fundamental distinction between SIAM and PAM. For SIAM, we have a different number of states for a strongly localized level and the conduction electron subsystem: the conduction band contains  $2N$  states, whereas the localized (s-type) level contains only two. The comparison of (137) and (135) shows clearly that this difficulty does not exist for PAM : the number of states both in the localized and itinerant subsystems are the same, i.e.  $2N$ .

This important difference between SIAM and PAM appears also when we calculate inelastic scattering or self-energy corrections. By analogy with the Hubbard model,<sup>32,79,81</sup> the equation of motion (133) for PAM can be transformed exactly to the scattering equation of the form (22). Then, we are able to write down explicitly the Dyson equation (23) and the exact expression for the self-energy  $M$  in the matrix form:

$$\hat{M}_{k\sigma}(\omega) = \begin{pmatrix} 0 & 0 \\ 0 & M_{22} \end{pmatrix}. \quad (138)$$

Here the matrix element  $M_{22}$  is of the form

$$M_{22} = M_{k\sigma}(\omega) = \frac{U^2}{N^2} \sum_{pqrs} \left( {}^{(ir)} \langle\langle f_{k+p\sigma} f_{p+q-\sigma}^\dagger f_{q-\sigma} f_{r-\sigma}^\dagger f_{r+s-\sigma} f_{k+s\sigma}^\dagger \rangle\rangle^{(ir)} \right)^{(p)}. \quad (139)$$

To calculate the self-energy operator (139) in a self-consistent way, we proceed by analogy with the Hubbard model. Then we find both the expressions for the self-energy operator<sup>32,79,81</sup> by iteration procedure.

## 11 Quasiparticle Many-Body Dynamics of TIAM

Let us see now how to apply the results of the preceding Sections for the case of TIAM Hamiltonian (7). The initial intention of Alexander and Anderson<sup>3</sup> was to extend the theory of localized magnetic states of solute atoms in metals to the case of a pair of neighboring magnetic atoms.<sup>8,40</sup> It was found that the simplified model based on the idea that the important interaction is the diagonal exchange integral in the localized state, which is exactly soluble in Hartree-Fock theory for isolated ions, is still soluble, and the solutions show both ferromagnetic and antiferromagnetic exchange mechanisms.

Contrary to that, our approach go beyond the Hartree-Fock approximation and permits one to describe the quasiparticle many-body dynamics of TIAM in a self-consistent way.

We again consider the relevant matrix Green function of the form (cf.(27))

$$\hat{G}(\omega) = \begin{pmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{pmatrix} = \begin{pmatrix} \langle\langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle c_{k\sigma} | f_{1\sigma}^\dagger \rangle\rangle & \langle\langle c_{k\sigma} | f_{2\sigma}^\dagger \rangle\rangle \\ \langle\langle f_{1\sigma} | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle f_{1\sigma} | f_{1\sigma}^\dagger \rangle\rangle & \langle\langle f_{1\sigma} | f_{2\sigma}^\dagger \rangle\rangle \\ \langle\langle f_{2\sigma} | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle f_{2\sigma} | f_{1\sigma}^\dagger \rangle\rangle & \langle\langle f_{2\sigma} | f_{2\sigma}^\dagger \rangle\rangle \end{pmatrix}. \quad (140)$$

The equation of motion for Green function (140) reads

$$\sum_p \begin{pmatrix} (\omega - \epsilon_p)\delta_{pk} & -V_{1p}\delta_{pk} & -V_{1p}\delta_{pk} \\ -V_{1p} & \frac{1}{N}(\omega - E_{0\sigma}) & -V_{12} \\ -V_{2p} & -V_{21} & \frac{1}{N}(\omega - E_{0\sigma}) \end{pmatrix} \begin{pmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + U \begin{pmatrix} 0 & 0 & 0 \\ \langle\langle A_1 | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle A_1 | f_{1\sigma}^\dagger \rangle\rangle & \langle\langle A_1 | f_{2\sigma}^\dagger \rangle\rangle \\ \langle\langle A_2 | c_{k\sigma}^\dagger \rangle\rangle & \langle\langle A_2 | f_{1\sigma}^\dagger \rangle\rangle & \langle\langle A_2 | f_{2\sigma}^\dagger \rangle\rangle \end{pmatrix}. \quad (141)$$

The notation are as follows

$$A_1 = f_{1\sigma} f_{1-\sigma}^\dagger f_{1-\sigma}; \quad A_2 = f_{2\sigma} f_{2-\sigma}^\dagger f_{2-\sigma}. \quad (142)$$

In a compact notation, the equation (141) has the form

$$\sum_p F(p, k) G_{pk}(\omega) = \hat{I} + U D_p(\omega). \quad (143)$$

We thus have the equation of motion (143) which is a complete analogue of the corresponding equations for the SIAM and PAM. After introducing the irreducible parts by analogy with the equation (28)

$$\begin{aligned} {}^{(ir)}\langle\langle f_{1\sigma} f_{1-\sigma}^\dagger f_{1-\sigma} | B \rangle\rangle_\omega &= \langle\langle f_{1\sigma} f_{1-\sigma}^\dagger f_{1-\sigma} | B \rangle\rangle_\omega - \langle n_{1-\sigma} \rangle \langle\langle f_{1\sigma} | B \rangle\rangle_\omega, \\ {}^{(ir)}\langle\langle f_{2\sigma} f_{2-\sigma}^\dagger f_{2-\sigma} | B \rangle\rangle_\omega &= \langle\langle f_{2\sigma} f_{2-\sigma}^\dagger f_{2-\sigma} | B \rangle\rangle_\omega - \langle n_{2-\sigma} \rangle \langle\langle f_{2\sigma} | B \rangle\rangle_\omega, \end{aligned} \quad (144)$$

and performing the second-time differentiation of the higher-order Green function, and introducing the relevant irreducible parts, the equation of motion (143) is rewritten in the form of Dyson equation (23). The definition of the generalized mean field Green function is as follows

$$\sum_p \begin{pmatrix} (\omega - \epsilon_p)\delta_{pk} & -V_{1p}\delta_{pk} & -V_{1p}\delta_{pk} \\ -V_{1p} & \frac{1}{N}(\omega - E_{0\sigma} - U n_{-\sigma}) & -V_{12} \\ -V_{2p} & -V_{21} & \frac{1}{N}(\omega - E_{0\sigma} - U n_{-\sigma}) \end{pmatrix} \times \begin{pmatrix} G_{11}^0 & G_{12}^0 & G_{13}^0 \\ G_{21}^0 & G_{22}^0 & G_{23}^0 \\ G_{31}^0 & G_{32}^0 & G_{33}^0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (145)$$



The matrix Green function (145) describes the mean-field solution of the TIAM Hamiltonian. The explicit solutions for diagonal elements of  $G^0$  are

$$\langle\langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle_\omega^0 = \left( \omega - \epsilon_k - \frac{|V_{1k}|^2}{\omega - (E_{0\sigma} - Un_{-\sigma})} - \Delta_{11}(k, \omega) \right)^{-1}, \quad (146)$$

$$\langle\langle f_{1\sigma} | f_{1\sigma}^\dagger \rangle\rangle_\omega^0 = \left( \omega - (E_{0\sigma} - Un_{-\sigma}) - S(\omega) - \Delta_{22}(k, \omega) \right)^{-1}, \quad (147)$$

$$\langle\langle f_{2\sigma} | f_{2\sigma}^\dagger \rangle\rangle_\omega^0 = \left( \omega - (E_{0\sigma} - Un_{-\sigma}) - S(\omega) - \Delta_{33}(k, \omega) \right)^{-1}. \quad (148)$$

Here we introduced the notation

$$\Delta_{11}(k, \omega) = \left( V_{2k} + \frac{V_{1k}V_{12}}{\omega - (E_{0\sigma} - Un_{-\sigma})} \right) \left( V_{2k} + \frac{V_{1k}V_{21}}{\omega - (E_{0\sigma} - Un_{-\sigma})} \right) \times \left[ \omega - (E_{0\sigma} - Un_{-\sigma}) - \frac{V_{21}V_{12}}{\omega - (E_{0\sigma} - Un_{-\sigma})} \right]^{-1}, \quad (149)$$

$$\Delta_{22}(k, \omega) = (\lambda_{21}(\omega) + V_{12})(\lambda_{21}(\omega) + V_{21}) \left[ \omega - (E_{0\sigma} - Un_{-\sigma}) - \frac{\sum_p |V_{2p}|^2}{\omega - \epsilon_p} \right]^{-1}, \quad (150)$$

$$\Delta_{33}(k, \omega) = (\lambda_{12}(\omega) + V_{21})(\lambda_{12}(\omega) + V_{12}) \left[ \omega - (E_{0\sigma} - Un_{-\sigma}) - \frac{\sum_p |V_{1p}|^2}{\omega - \epsilon_p} \right]^{-1}, \quad (151)$$

$$\lambda_{12} = \lambda_{21} = \sum_p \frac{V_{1p}V_{2p}}{\omega - \epsilon_p}. \quad (152)$$

The formal solution of the Dyson equation for TIAM contains the self-energy matrix

$$\hat{M} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & M_{22} & M_{23} \\ 0 & M_{32} & M_{33} \end{pmatrix}, \quad (153)$$

where

$$M_{22} = U^2 \langle\langle f_{1\sigma} n_{1-\sigma} | f_{1\sigma}^\dagger n_{1-\sigma} \rangle\rangle^{(ir)p}, \quad (154)$$

$$M_{32} = U^2 \langle\langle f_{2\sigma} n_{2-\sigma} | f_{1\sigma}^\dagger n_{1-\sigma} \rangle\rangle^{(ir)p}, \quad (155)$$

$$M_{23} = U^2 \langle\langle f_{1\sigma} n_{1-\sigma} | f_{2\sigma}^\dagger n_{2-\sigma} \rangle\rangle^{(ir)p}, \quad (156)$$

$$M_{33} = U^2 \langle\langle f_{2\sigma} n_{2-\sigma} | f_{2\sigma}^\dagger n_{2-\sigma} \rangle\rangle^{(ir)p}. \quad (157)$$

To calculate the matrix elements (154), the same procedure can be used as it was done previously for the SIAM (44). As a result, we find the following explicit expressions for the self-energy matrix

elements (cf.(46))

$$M_{22}^{\uparrow}(\omega) = U^2 \int_{-\infty}^{+\infty} d\omega_1 d\omega_2 \frac{1 + N(\omega_1) - n(\omega_2)}{\omega - \omega_1 - \omega_2} \times \left( -\frac{1}{\pi} \text{Im} \langle \langle S_1^- | S_1^+ \rangle \rangle_{\omega_1} \right) \left( -\frac{1}{\pi} \text{Im} \langle \langle f_{1\downarrow} | f_{1\downarrow}^\dagger \rangle \rangle_{\omega_2} \right), \quad (158)$$

$$M_{22}^{\downarrow}(\omega) = U^2 \int_{-\infty}^{+\infty} d\omega_1 d\omega_2 \frac{1 + N(\omega_1) - n(\omega_2)}{\omega - \omega_1 - \omega_2} \times \left( -\frac{1}{\pi} \text{Im} \langle \langle S_1^+ | S_1^- \rangle \rangle_{\omega_1} \right) \left( -\frac{1}{\pi} \text{Im} \langle \langle f_{1\uparrow} | f_{1\uparrow}^\dagger \rangle \rangle_{\omega_2} \right), \quad (159)$$

$$M_{23}^{\uparrow}(\omega) = U^2 \int_{-\infty}^{+\infty} d\omega_1 d\omega_2 \frac{1 + N(\omega_1) - n(\omega_2)}{\omega - \omega_1 - \omega_2} \times \left( -\frac{1}{\pi} \text{Im} \langle \langle S_1^- | S_2^+ \rangle \rangle_{\omega_1} \right) \left( -\frac{1}{\pi} \text{Im} \langle \langle f_{1\downarrow} | f_{2\downarrow}^\dagger \rangle \rangle_{\omega_2} \right), \quad (160)$$

$$M_{23}^{\downarrow}(\omega) = U^2 \int_{-\infty}^{+\infty} d\omega_1 d\omega_2 \frac{1 + N(\omega_1) - n(\omega_2)}{\omega - \omega_1 - \omega_2} \times \left( -\frac{1}{\pi} \text{Im} \langle \langle S_2^+ | S_1^- \rangle \rangle_{\omega_1} \right) \left( -\frac{1}{\pi} \text{Im} \langle \langle f_{1\uparrow} | f_{2\uparrow}^\dagger \rangle \rangle_{\omega_2} \right). \quad (161)$$

Here the following notation were used:

$$S_i^+ = f_{i\uparrow}^\dagger f_{i\downarrow}; \quad S_i^- = f_{i\downarrow}^\dagger f_{i\uparrow}; \quad i = 1, 2.$$

For  $M_{33}$  we obtain the same expressions as for  $M_{22}$  with the substitution of index 1 by 2. For  $M_{32}^{\uparrow\downarrow}$  we must do the same. It is possible to say that the diagonal elements  $M_{22}$  and  $M_{33}$  describe single-site inelastic scattering processes; off-diagonal elements  $M_{23}$  and  $M_{32}$  describe intersite inelastic scattering processes. They are responsible for the specific features of the dynamic behavior of TIAM ( as well as the off-diagonal matrix elements of the Green function  $G^0$ ) and, more generally, the cluster impurity Anderson model (CIAM). The nonlocal contributions to the total spin susceptibility of two well formed impurity magnetic moments at a distance  $R$  can be estimated as

$$\chi_{pair} \sim \langle \langle S_1^- | S_2^+ \rangle \rangle \sim 2\chi - 12\pi E_F \left( \frac{\chi}{g\mu_B} \right)^2 \frac{\cos(2k_F R)}{(k_F R)^3}. \quad (162)$$

In the region of interplay of the RKKY and Kondo behavior, the key point is then to connect the partial Kondo screening effects with the low temperature behavior of the total spin susceptibility. As it is known, it is quite difficult to describe such a threshold behavior analytically. However, progress is expected due to a better understanding of the quasiparticle many-body dynamics both from analytical and numerical investigations.

## 12 Conclusions

In summary, we presented in this paper in terse form a general technique how a dynamical solution for SIAM and TIAM at finite temperatures and for the broad interval of the values of the model parameters can be constructed in the spirit of irreducible Green functions approach. We used an exact result to connect the single-particle Green function with the higher-order Green function to obtain an complex expansion in terms of  $U$  and  $V$  for the propagator. This approach provides a plausible yet sound understanding of how structure of the relevant dynamical solution may be found. Hence this approach offer a both powerful and workable technique for a systematic construction of the approximative dynamical solutions of SIAM, PAM and other models of the

strongly correlated electron systems.

In short, the theory of the many-body quasiparticle dynamics of the Anderson- and Hubbard-type models at finite temperatures have been reviewed. We stressed an importance of the new **exact identity** relating the one-particle and many-particle Green functions for the single-impurity Anderson model:  $G = g_0 + g_0 P g_0$ .

The application of the IGF method to the investigation of nonlocal correlations and quasiparticle interactions in Anderson models<sup>8</sup> has a particular interest for studying of the inter-site correlation effects in the concentrated Kondo system and other problems of solid state physics.<sup>40,65</sup> A comparative study of real many-body dynamics of single-impurity, two-impurity, and periodic Anderson model, especially for strong but finite Coulomb correlation, when perturbation expansion in  $U$  does not work, is of importance for the characterization of the true quasiparticle excitations and the role of magnetic correlations. It was shown that the physics of two-impurity Anderson model can be understood in terms of competition between itinerant motion of carriers and magnetic correlations of the RKKY nature. This issue is still very controversial and the additional efforts must be applied in this field.

The many-body quasiparticle dynamics of the single-impurity Anderson Model was investigated by means of the equations of motion for the higher-order Green functions. It was shown that an interpolating approximation, which simultaneously reproduces the weak-coupling limit up to second order in the interaction strength  $U$  and the strong coupling limit up to second order in the hybridization  $V$  (and thus also fulfills the atomic limit) may be formulated self-consistently. Hence, a new advanced many-body dynamical solution for SIAM has been developed, which recovers the exactly solvable limits  $V = 0$  and  $U = 0$  and which is even more at least correct up to order  $V^2$  in a strong-coupling expansion and simultaneously up to order  $U^2$  in a weak-coupling expansion.

Further applications and development of the technique of the equations of motion for the Green functions were described in Refs.<sup>34,86,87,88,89,90,91,92,93,94,95</sup> These applications illustrate some of subtle details of this approach and exhibit the physical significance and operational ability of the Green function technique in a representative form.

This line of consideration is very promising for developing the complete and self-contained theory of strongly interacting many-body systems on a lattice.<sup>5,6,7,8,9,10,11,12,32,78,79,80,81,82,83,84,85</sup> Our main results reveal the fundamental importance of the adequate definition of *generalized mean fields* at finite temperatures, that results in a deeper insight into the nature of quasiparticle states of the correlated lattice fermions and spins. We believe that our approach offers a new way for systematic constructions of the approximate dynamic solutions of the Hubbard, SIAM, TIAM, PAM, spin-fermion, and other models of the strongly correlated electron systems on a lattice.

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