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QUASIPARTICLE MANY-BODY DYNAMICS OF THE ANDERSON MODEL

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The paper addresses the many-body quasiparticle dynamics of the Anderson impurity model at finite temperatures in the framework of the equation-of-motion method. We find a new exact identity relating the one-particle and many-particle Green's functions. Using this identity we present a consistent and general scheme for a construction of generalized mean fields (elastic scattering corrections) and self-energy (inelastic scattering) in terms of Dyson equation. A new approach for the complex expansion for the single-particle propagator in terms of Coulomb repulsion U and hybridization V is proposed. Using the exact identity, the essentially new many-body dynamical solution of SIAM has been derived. This approach offers a new way for the systematic construction of the approximative interpolating dynamical solutions of the strongly correlated electron systems.

1. Introduction

The study of the quasiparticle excitations in solids has been one of the most fascinating subjects for many years.[1] The subject of the present paper is a microscopic many-body theory of strongly correlated electron models. A principal importance of this problem is related with the dual character of electrons in a wide class of materials (transition metal oxides, intermediate-valence solids, heavy fermions and high-T_c superconductors). The behavior of electrons in these materials exhibit both localized and delocalized features.[2] Contrary to the wide-band electron systems (like simple metals), where the fundamentals are very well known and the electrons can be represented in a way such that they weakly interact with each other, in these substances the bands are narrow, the electrons interact strongly and moreover their spectra are complicated.

The problem of the adequate description of the strongly correlated electron systems has been studied intensively during the last decade, especially in context of Heavy Fermions and High-T_c superconductivity.[2] The understanding of the true nature of the electronic states and their quasiparticle dynamics are one of the central topics of the current experimental and theoretical efforts in the field. The

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plenty of experimental and theoretical results show that this many-body quasiparticle dynamics is quite nontrivial. A vast amount of theoretical searches for the suitable description of the strongly correlated fermion systems deal with the simplified model Hamiltonians. These include as workable patterns single-impurity Anderson model (SIAM)[3] and Hubbard model.[4] In spite of certain drawbacks these models exhibit the key physical feature: the competition and interplay between kinetic energy (itinerant) and potential energy (localized) effects. A fully consistent theory of quasiparticle dynamics of both models is believed to be crucially important[5,6] for a deeper understanding of the true nature of the electronic states in the above mentioned class of materials.

In spite of many theoretical efforts the complete solution of dynamical problem still lacking for the "simple" Anderson/Hubbard model. One of the main reasons for this is that it has been recognized relatively recently only[7] that the simplicity of the Anderson model manifests itself not in the many-body dynamics (the right definition of the quasiparticles via the poles of the Green's functions) but rather at quite different level — in the dynamics of the two-particle scattering, resulting in the elegant Bethe-ansatz solution, which gives the static characteristics (static susceptibility, specific heat etc.). In this sense, as to the true many-body dynamics, the complete analytical solution of this problem is still a quite open subject. The present paper is primarily devoted to the analysis of the relevant many-body dynamical solution of the SIAM and its correct functional structure. We wish to determine which solution actually arise from both the self-consistent many-body approach and intrinsic nature of the model itself. We believe strongly that before numerical calculations of the spectral intensity of the Green function at low energy and low temperature it is quite important to have the consistent and close analytical representation for the one-particle GF of SIAM and Hubbard model. To confirm this let us mention two examples only: (i) recent "exact" dynamical solution[8] of the Anderson model, which is in fact the well-known lowest order approximative interpolation solution[9]; (ii) "nonperturbative" self-energy corrections to the Hubbard model,[10] where the self-energy [Eq. (15)] in the second-order in U (cf. Ref. 5) has been used for the calculation of the corrections to "Hubbard I" solution, which is essentially strong-U solution and, moreover, is incorrect even in this limit. A proper many-body description of dynamic correlations is very actual also for the investigation of the dynamics of many-impurity Anderson model, where standard advanced many-body methods does not work properly in usual formulation. Recently, a lot of efforts have been devoted for better understanding of the static and dynamical properties of the Anderson Model in the context of many impurity case (e.g. Refs. 6 and 11). This field is quite important for description of magnetic properties of anomalous rare-earth compounds.[12–16] Although the few-impurity Anderson model has not been studied extensively, with the use of conformal field theories the corresponding Kondo problem has been at this point clarified substantially.[17]

The problem of an adequate and consistent description of dynamics of single-impurity and many-impurity Anderson models (SIAM and TIAM) and other models

of correlated lattice electrons is still not completely solved analytically. It is well known,[1] that the proper theoretical description of the dynamical properties of the Anderson model has a direct relationship with experiment, namely with different types of photoelectronic studies of f and d electrons in rare-earths and actinide compounds,[18,19] and description of transport properties. Core-level X-ray photoemission and photoabsorption spectroscopies are powerful tools in the study of electron states in solids. The Anderson model provides a microscopic basis and also a point of view for discussing this phenomena.[20] There are some points still open to discussion in this field[21,22] and to settle this issue we need a better understanding, a first-principles microscopic description of the many-body quasiparticle dynamics of the Anderson and related models. This problem has been studied intensively during last decades.[23–30] The paper[30] clearly shows the importance of the calculation of the Green's function and spectral densities in a self-consistent way. A remarkable achievement was made recently in papers[31,32] with numerical renormalization group approach. Their results, though being only numerical, provide an accurate description for the frequency and temperature dependence of the single-particle spectral densities and transport time.

During the last decades a lot of theoretical papers have been published, attacking the Anderson model by many refined many-body analytical methods.[33–43] Nevertheless, the fully consistent dynamical analytical solution in the closed form for a single-particle propagator of SIAM is still lacking. In this paper the problem of consistent analytical description of the many-body dynamics of SIAM will be discussed in the framework of equation-of-motion appproach for two-time thermodynamic Green's functions. Our main motivation was the fact that an interesting approach to dynamics of the Anderson model[36,37] (and Hubbard model[10]) was formulated recently using the modified version of Kadanoff–Baym method. Our aim is to compare this approach with the equation-of-motion technique for two-time thermodynamic Green's functions, having in mind to find the most suitable technique for subsequent description of a dynamics of few-impurity Anderson model.

2. Model

The Hamiltonian of SIAM can be written in the form

$$H = \sum_{k\sigma} \epsilon_k c^+_{k\sigma} c_{k\sigma} + \sum_{\sigma} E_{0\sigma} f^+_{0\sigma} f_{0\sigma} + \frac{U}{2} \sum_{\sigma} n_{0\sigma} n_{0-\sigma} + \sum_{k\sigma} V_k (c^+_{k\sigma} f_{0\sigma} + f^+_{0\sigma} c_{k\sigma}) , \tag{1}$$

where $c^+_{k\sigma}$ and $f^+_{0\sigma}$ are respectively the creation operators for conduction and localized electrons; ϵ_k is the conduction electron energy, $E_{0\sigma}$ is the localized electron energy level and U is the intra-atomic Coulomb interaction at the impurity site. V_k represents the s–f hybridization.

Our goal is to propose the new combined many-body approach for description of the many-body quasiparticle dynamics of SIAM at finite temperatures. The interplay and competition of the kinetic energy (ϵ_k), potential energy (U) and hybridization (V) affects substantially the electronic spectrum. The renormalized electron energies are temperature dependent and electronic states have a finite life times. These effects are most suitable accounted for the Green functions method.[1,2] The way of derivation of the "exact" solution[8] gives to us an opportunity to emphasize some important issues about the relevant dynamical solutions of the strongly correlated electron models (SIAM, TIAM, Hubbard model, PAM etc.) and to formulate in a more sharp form the ideas of the method of the Irreducible Green's Functions (IGF).[5] This IGF method allows one to describe the quasiparticle spectra with damping of the strongly correlated electron systems in a very general and natural way and to construct the relevant dynamical solution in a self-consistent way on the level of Dyson equation without decoupling the chain of the equation of motion for the GFs.

3. Dynamical Properties

At this point it is worthwhile to underline that despite that the fully consistent dynamical solution of SIAM is still lacking, a few important contributions has been done previously with the equations of motion for the GFs. To give a more instructive discussion let us consider the single-particle GF of localized electrons, which is defined as

$$\begin{aligned} G_\sigma(t) &= \langle\langle f_{0\sigma}(t), f_{0\sigma}^+ \rangle\rangle \\ &= -i\theta(t)\langle [f_{0\sigma}(t), f_{0\sigma}^+]_+ \rangle \\ &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega \exp(-i\omega t) G_\sigma(\omega)\,. \end{aligned} \tag{2}$$

The simplest approximative "interpolating" solution of SIAM has the form[9]:

$$\begin{aligned} G_\sigma(\omega) &= \frac{1}{\omega - E_{0\sigma} - S(\omega)} + \frac{U\langle n_{0-\sigma}\rangle}{(\omega - E_{0\sigma} - S(\omega) - U)(\omega - E_{0\sigma} - S(\omega))} \\ &= \frac{1 - \langle n_{0-\sigma}\rangle}{\omega - E_{0\sigma} - S(\omega)} + \frac{\langle n_{0-\sigma}\rangle}{\omega - E_{0\sigma} - S(\omega) - U}\,, \end{aligned} \tag{3}$$

where

$$S(\omega) = \sum_k \frac{|V_k|^2}{\omega - \epsilon_k}\,. \tag{4}$$

The values of n_σ should to be determined through the self-consistency equation

$$n_\sigma = \langle n_{0\sigma}\rangle = -\frac{1}{\pi}\int dE\, f(E)\mathrm{Im}\, G_\sigma(E, n_\sigma)\,, \tag{5}$$

where

$$f(E) = [\exp(\beta E) + 1]^{-1} .$$

This solution is valid at small V only and was analyzed in detail in Ref. 24 in the context of screening effects in the core-level spectra of mixed-valence compounds, where it was shown that solution (3) is valid for $V < 0.5$ eV (with core-hole interaction). The "atomic-like" interpolating solution (3) reproduces correctly the two important limits:

$$\begin{aligned} G_\sigma(\omega) &= \frac{1 - \langle n_{0-\sigma}\rangle}{\omega - E_{0\sigma}} + \frac{\langle n_{0-\sigma}\rangle}{\omega - E_{0\sigma} - U} , \quad \text{for} \quad V = 0 \\ G_\sigma(\omega) &= \frac{1}{\omega - E_{0\sigma} - S(\omega)} , \qquad\qquad \text{for} \quad U = 0 . \end{aligned} \tag{6}$$

The important point about formulas (6) is that any approximate solution of SIAM should be consistent with it. Let us remind how to get solution (3). It follows from the system of equation for small-V limit:

$$(\omega - E_{0\sigma} - S(\omega))\langle\langle f_{0\sigma}|f^+_{0\sigma}\rangle\rangle_\omega = 1 + U\langle\langle f_{0\sigma}n_{0-\sigma}|f^+_{0\sigma}\rangle\rangle_\omega , \tag{7}$$

$$(\omega - E_{0\sigma} - U)\langle\langle f_{0\sigma}n_{0-\sigma}|f^+_{0\sigma}\rangle\rangle_\omega \approx \langle n_{0-\sigma}\rangle + \sum_k V_k\langle\langle c_{k\sigma}n_{0\sigma}|f^+_{0\sigma}\rangle\rangle_\omega , \tag{8}$$

$$(\omega - \epsilon_k)\langle\langle c_{k\sigma}n_{0-\sigma}|f^+_{0\sigma}\rangle\rangle_\omega = V_k\langle\langle f_{0\sigma}n_{0-\sigma}|f^+_{0\sigma}\rangle\rangle_\omega . \tag{9}$$

The equation (8) is approximative; it include two more terms, which were threated in the limit of small V in Ref. 34. The solution (3) has been obtained in Ref. 8 and presented as an "exact". We shall see later on that, in fact, all results in Ref. 8 are approximative and are valid in the lowest order in V.

Another advanced many-body approach to analytical solution of SIAM was proposed in Ref. 36. A modified Kadanoff–Baym equation-of-motion technique has been used in Ref. 36 to get a solution, which have a number of truly remarkable properties. This solution was first found analytically,[36] then only recently verified numerically.[37] To find more complex expansion, including both U and V, the "mean-fields" in Ref. 36 were "introduced" as follows:

$$\begin{aligned} \langle\langle f_{0\sigma}f^+_{0-\sigma}c_{k-\sigma}|f^+_{0\sigma}\rangle\rangle &\approx \langle f^+_{0-\sigma}c_{k-\sigma}\rangle\langle\langle f_{0\sigma}|f^+_{0\sigma}\rangle\rangle , \\ \langle\langle f_{0\sigma}c^+_{k-\sigma}f_{0-\sigma}|f^+_{0-\sigma}\rangle\rangle &\approx \langle c^+_{k-\sigma}f_{0-\sigma}\rangle\langle\langle f_{0\sigma}|f^+_{0\sigma}\rangle\rangle , \\ \langle\langle c_{k\sigma}f^+_{0-\sigma}c_{p-\sigma}|f^+_{0\sigma}\rangle\rangle &\approx \langle f^+_{0-\sigma}c_{p-\sigma}\rangle\langle\langle c_{k\sigma}|f^+_{0\sigma}\rangle\rangle , \\ \langle\langle c_{k\sigma}c^+_{p-\sigma}f_{0-\sigma}|f^+_{0\sigma}\rangle\rangle &\approx \langle c^+_{p-\sigma}f_{0-\sigma}\rangle\langle\langle c_{k\sigma}|f^+_{0\sigma}\rangle\rangle . \end{aligned} \tag{10}$$

In fact, the procedure of introduction of the mean field corrections in Ref. 36 remind (but not coincide) with that of the more systematic IGF method. The inelastic scattering corrections (self-energy) and elastic ones (mean-field) are separated in

the IGF method in the most consistent and general way. The Neal's definition (10) will be clearer if one rewrite the "effective mean-field" part of the full Neal's solution in the following form

$$G_\sigma = \frac{1}{\omega - E_{0\sigma} - S(\omega) - Z_\sigma(\omega)} + \frac{Un_{-\sigma}}{(\omega - E_{0\sigma} - S(\omega) - U)(\omega - E_{0\sigma} - S(\omega) - Z_\sigma(\omega))}. \tag{11}$$

Here

$$Z_\sigma = \frac{U}{\omega - E_{0\sigma} - S(\omega) - U}\left(1 + \sum_k \frac{|V_k|^2}{(\omega - \epsilon_k)^2}\right) \times \left[\sum_p V_p(\langle f^+_{0-\sigma} c_{p-\sigma}\rangle - \langle c^+_{p-\sigma} f_{0-\sigma}\rangle)\right]. \tag{12}$$

Since the symmetry properties of $\langle c^+_{k\sigma} f_{0\sigma}\rangle$, the connection of the GFs (11) and (3) can now be made by noting that $Z_\sigma = 0$.

4. Generalized Mean Fields

We now proceed to the details. In the important paper[34] the calculation of the GF (2) has been considered in the limit of infinitely strong Coulomb correlation U and small hybridization V. It was shown, with the using the decoupling procedure for the higher-order GFs, that the obtained solution gives the correct result in the Kondo limit at low temperatures and for some other limits. The functional structure of the Lacroix's solution generalize the solution (3). The Ref. 34 deals with the GF (2). The starting point is the system of equations:

$$(\omega - E_{0\sigma} - S(\omega))\langle\langle f_{0\sigma}|f^+_{0\sigma}\rangle\rangle = 1 + U\langle\langle f_{0\sigma} n_{0-\sigma}|f^+_{0\sigma}\rangle\rangle, \tag{13}$$

$$(\omega - E_{0\sigma} - U)\langle\langle f_{0\sigma} n_{0-\sigma}|f^+_{0\sigma}\rangle\rangle = \langle n_{0-\sigma}\rangle + \sum_k V_k(\langle\langle c_{k\sigma} n_{0-\sigma}|f^+_{0\sigma}\rangle\rangle - \langle\langle c_{k-\sigma} f^+_{0-\sigma} f_{0\sigma}|f^+_{0\sigma}\rangle\rangle + \langle\langle c^+_{k-\sigma} f_{0\sigma} f_{0-\sigma}|f^+_{0\sigma}\rangle\rangle). \tag{14}$$

Using the relatively simple decoupling procedure for higher-order equation of motion, the qualitatively correct low-temperature spectral intensity has been calculated. The final expression for the GF (2) for finite U has the form

$$\langle\langle f_{0\sigma}|f^+_{0\sigma}\rangle\rangle = \frac{1}{\omega - E_{0\sigma} - S(\omega) + US_1(\omega)} + \frac{U\langle n_{0-\sigma}\rangle + UF_1(\omega)}{K(\omega)(\omega - E_{0\sigma} - S(\omega) + US_1(\omega))}, \tag{15}$$

where F_1, S_1 and K are certain complicated expressions, which can be easily derived. We shall write down explicitly the infinite U approximate GF[34]:

$$\langle\langle f_{0\sigma}|f^+_{0\sigma}\rangle\rangle = \frac{1-\langle n_{0-\sigma}\rangle - F_\sigma(\omega)}{\omega - E_{0\sigma} - S(\omega) - Z^1_\sigma(\omega)}\,. \tag{16}$$

The following notations have been used

$$F_\sigma = V\sum_k \frac{\langle f^+_{0-\sigma}c_{k-\sigma}\rangle}{\omega-\epsilon_k}\,, \tag{17}$$

$$Z^1_\sigma = V^2\sum_{q,k}\frac{\langle c^+_{q-\sigma}c_{k-\sigma}\rangle}{\omega-\epsilon_k} - S(\omega)V\sum_k\frac{\langle f^+_{0-\sigma}c_{k-\sigma}\rangle}{\omega-\epsilon_k}\,. \tag{18}$$

The functional structure of the single-particle GF (16) is quite transparent. The expression in numerator of (16) plays a role of "dynamical mean-field," which is proportional to $\langle f^+_{0-\sigma}c_{k-\sigma}\rangle$. In the denominator instead of bare shift $S(\omega)$ (4) we have an "effective shift" $S^1 = S(\omega) + Z^1_\sigma(\omega)$. The choice of the specific procedure of decoupling for the higher-order equation of motion specify the selected "generalized mean fields" (GMFs) and "effective shifts." This is a central statement of the present considerations which we shall illustrate below in detail.

5. Interpolating Solution

It will be quite revealing to discuss briefly the general concepts of constructing of interpolative dynamical solution of the strongly correlated electron models. The very problem of the consistent interpolation solution of the many-body electron models was formulated explicitly by Hubbard[44] in the context of Hubbard model and by Kim[45] in context of SIAM. Hubbard clearly pointed out one particular feature of consistent theory, insisting that it should give exact results in the two opposite limits of very wide and very narrow bands. It was argued by Hubbard,[44] "that this was a desirable feature of a theory which was intended to interpolate between these limits." The same remarks were made by Kim[45] for SIAM.

The functional structure of required interpolating solution can be clarified if one considers the atomic (very narrow band) solution of the Hubbard model:

$$G^{\rm at}(\omega) = \frac{1-n_{-\sigma}}{\omega - t_0} + \frac{n_{-\sigma}}{\omega - t_0 - U} = \frac{1}{\omega - t_0 - \Sigma^{\rm at}(\omega)} \tag{19}$$

where

$$\Sigma^{\rm at}(\omega) = \frac{n_{-\sigma}U}{1-\frac{(1-n_{-\sigma})U}{\omega-t_0}}\,. \tag{20}$$

Let us consider the expansion in terms of U:

$$\Sigma^{\rm at}(\omega) \approx n_{-\sigma}U + n_{-\sigma}(1-n_{-\sigma})U^2\frac{1}{\omega-t_0} + O(U)\,. \tag{21}$$

The well-known "Hubbard I" solution can be written as

$$G_k = \frac{1}{\omega - \epsilon(k) - \Sigma^{\mathrm{at}}(\omega)} = \frac{1}{(G^{\mathrm{at}})^{-1} + t_0 - \epsilon(k)}. \tag{22}$$

The partial "Hubbard III" solution, which called "alloy analogy" approximation has the form:

$$\Sigma(\omega) = \frac{n_{-\sigma}U}{1 - (U - \Sigma(\omega))G(\omega)}. \tag{23}$$

Equation (23) is possible to get from (20) taking into account the following relationship:

$$\frac{1}{\omega - t_0} \propto \frac{1}{1 - n_{-\sigma}} G(\omega) - \Sigma(\omega)G(\omega). \tag{24}$$

The Coherent Potential Approximation (CPA) provides a basis for physical interpretation of equation (23), which correspond to elimination of the dynamics of $-\sigma$ electrons. In analogy with (21) it is possible to expand:

$$\frac{n_{-\sigma}U}{1 - (U - \Sigma(\omega))G(\omega)} \approx n_{-\sigma}U + n_{-\sigma}U(U - \Sigma)G^0(\omega - \Sigma) + O(U). \tag{25}$$

The solution (16) does not reproduce correctly the U-perturbation expansion (cf. Ref. 41) for the self-energy of the GF (2):

$$\begin{aligned} M_\sigma(\omega) \sim U\langle n_{0-\sigma}\rangle + U^2 \int dE_1 \int dE_2 \\ \times \int dE_3 \frac{f(E_1)f(E_2)(1 - f(E_3)) + (1 - f(E_1)(1 - f(E_2))f(E_3)}{\omega - E_1 - E_2 + E_3} \\ \times \mathrm{Im}\, G_\sigma(E_1)\mathrm{Im}\, G_{-\sigma}(E_2)\mathrm{Im}\, G_{-\sigma}(E_3). \end{aligned} \tag{26}$$

It will be shown in separate publication elsewhere that it is possible to find certain way to incorporate this U^2 perturbation theory expansion in the functional structure of the interpolating dynamical solution of SIAM in a self-consistent way on the level of the higher-order GFs. A heuristic semi-empirical approach for constructing such a solution for SIAM and periodic Anderson Model (PAM) has been proposed in Ref. 39 and for Hubbard model in Ref. 46. The advanced many-body dynamical solution of papers,[36,37] which correctly reproduces (6), does not incorporate (in one expression) (26), too. The IGF approach[5,41] with the using of minimal algebra of relevant operators allows one to find an interpolating solution for weak and strong Coulomb interaction U and to calculate explicitly the quasiparticle spectra and their damping for both limits. The U-perturbation expansion (26) is included in the IGF scheme in a self-consistent way. That means that one can use the suitable iteration procedure for the system of equations[41]:

$$\langle\langle f_{0\sigma}|f_{0\sigma}^{+}\rangle\rangle = \frac{1}{\omega - E_{0\sigma} - Un_{-\sigma} - S(\omega) - M_{00}^{\sigma}}, \tag{27}$$

$$M_{00}^{\sigma} \approx U^2 \int_{-\infty}^{+\infty} \frac{dE_1 dE_2 dE_3}{\omega + E_1 - E_2 - E_3} \Big[f(E_1)(1 - f(E_2) - f(E_3)) + f(E_2)f(E_3) \Big] g_{0-\sigma}(E_1) g_{0\sigma}(E_2) g_{0-\sigma}(E_3), \tag{28}$$

$$g_{0\sigma} = -\frac{1}{\pi} \mathrm{Im} \langle\langle f_{0\sigma}|f_{0\sigma}^{+}\rangle\rangle. \tag{29}$$

If we take for the first iteration step in (28)

$$g_{0\sigma} \simeq \delta(E - E_{0\sigma} - Un_{-\sigma}), \tag{30}$$

we obtain

$$M_{00}^{\sigma}(\omega) = U^2 \frac{f(E_{0\sigma} + Un_{-\sigma})(1 - f(E_{0\sigma} + Un_{-\sigma}))}{\omega - E_{0\sigma} - Un_{-\sigma}} = U^2 N_{-\sigma}(1 - N_{-\sigma}) G_{\sigma}^{0}(\omega), \tag{31}$$

where $N_{-\sigma} = f(E_{0\sigma} + Un_{-\sigma})$. This is well known "atomic" limit of the self-energy in the sense of equation (25). The correct second-order contribution in the local approximation for the Hubbard model has the form[46]

$$\tilde{G}_{\sigma} \propto \frac{G_{\sigma} \langle\langle n_{0-\sigma}|n_{0-\sigma}\rangle\rangle}{n_{-\sigma}(1 - n_{-\sigma})}. \tag{32}$$

The same arguments should be valid for SIAM too.

6. Complex Expansion for a Propagator

We now proceed with analytical many-body consideration. One may attempt to consider the suitable solution for the SIAM starting from the following exact relation, which was derived in Ref. 41:

$$\langle\langle f_{0\sigma}|f_{0\sigma}^{+}\rangle\rangle = g^0 + g^0 P g^0, \tag{33}$$

$$g^0 = (\omega - E_{0\sigma} - S(\omega))^{-1}, \tag{34}$$

$$P = U\langle n_{0-\sigma}\rangle + U^2 \langle\langle f_{0\sigma} n_{0-\sigma}|f_{0\sigma}^{+} n_{0-\sigma}\rangle\rangle. \tag{35}$$

The advantage of the equation (33) is that it is purely identity and does not include any approximation. Having emphasized the importance of the role of the equation (33), let us see now what is the best possible fit for the higher-order GF in (35). We proceed by considering the equation of motion for it:

$$(\omega - E_{0\sigma} - U)\langle\langle f_{0\sigma} n_{0-\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle$$

$$= \langle n_{0-\sigma}\rangle + \sum_{k} V_k(\langle\langle c_{k\sigma} n_{0-\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle$$

$$+ \langle\langle c^{+}_{k-\sigma} f_{0\sigma} f_{0-\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle - \langle\langle c_{k-\sigma} f^{+}_{0-\sigma} f_{0\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle). \quad (36)$$

We can think of it as defining the new kinds of elastic and inelastic scattering processes that contribute to the formation of the generalized mean fields and self-energy (damping) corrections. The construction of the suitable mean fields can be quite nontrivial[5,6] and it is rather difficult to get it from an intuitive physical point of view. To describe these contributions self-consistently let us consider, in analogy with Ref. 34, the equations of motion for the higher-order GFs in the R.H.S. of (36).

$$(\omega - \epsilon_k)\langle\langle c_{k\sigma} n_{0-\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle$$

$$= V\langle\langle f_{0\sigma} n_{0-\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle + \sum_{p} V(\langle\langle c_{k\sigma} f^{+}_{0-\sigma} c_{p-\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle$$

$$- \langle\langle c_{k\sigma} c^{+}_{p-\sigma} f_{0-\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle), \quad (37)$$

$$(\omega - \epsilon_k - E_{0\sigma} + E_{0-\sigma})\langle\langle c_{k-\sigma} f^{+}_{0-\sigma} f_{0\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle$$

$$= -\langle f^{+}_{0-\sigma} c_{k-\sigma} n_{0\sigma}\rangle - V\langle\langle f_{0\sigma} n_{0-\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle$$

$$+ \sum_{p} V(\langle\langle c_{k-\sigma} f^{+}_{0-\sigma} c_{p\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle$$

$$- \langle\langle c_{k-\sigma} c^{+}_{p-\sigma} f_{0\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle), \quad (38)$$

$$(\omega + \epsilon_k - E_{0\sigma} - E_{0-\sigma} - U)\langle\langle c^{+}_{k-\sigma} f_{0\sigma} f_{0-\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle$$

$$= -\langle c^{+}_{k-\sigma} f_{0\sigma} f^{+}_{0\sigma} f_{0-\sigma}\rangle + V\langle\langle f_{0\sigma} n_{0-\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle$$

$$+ \sum_{p} V(\langle\langle c^{+}_{k-\sigma} c_{p\sigma} f_{0-\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle$$

$$+ \langle\langle c^{+}_{k-\sigma} f_{0\sigma} c_{p-\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle). \quad (39)$$

Now let us see how to proceed forth to get the suitable functional structure of the relevant solution. The intrinsic nature of the system of the equations of motion (37)–(39) suggest to consider the following approximation:

$$(\omega - \epsilon_k)\langle\langle c_{k\sigma} n_{0-\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle \approx V\langle\langle f_{0\sigma} n_{0-\sigma} | f^{+}_{0\sigma} n_{0-\sigma}\rangle\rangle, \quad (40)$$

$$(\omega - \epsilon_k - E_{0\sigma} + E_{0-\sigma})\langle\langle c_{k-\sigma} f^+_{0-\sigma} f_{0\sigma} | f^+_{0\sigma} n_{0-\sigma}\rangle\rangle$$
$$\approx -\langle f^+_{0-\sigma} c_{k-\sigma} n_{0\sigma}\rangle - V(\langle\langle f_{0\sigma} n_{0-\sigma} | f^+_{0\sigma} n_{0-\sigma}\rangle\rangle$$
$$- \langle\langle c_{k-\sigma} c^+_{k-\sigma} f_{0\sigma} | f^+_{0\sigma} n_{0-\sigma}\rangle\rangle)\,, \tag{41}$$

$$(\omega + \epsilon_k - E_{0\sigma} - E_{0-\sigma} - U)\langle\langle c^+_{k-\sigma} f_{0\sigma} f_{0-\sigma} | f^+_{0\sigma} n_{0-\sigma}\rangle\rangle$$
$$\approx -\langle c^+_{k-\sigma} f_{0\sigma} f^+_{0\sigma} f_{0-\sigma}\rangle + V(\langle\langle f_{0\sigma} n_{0-\sigma} | f^+_{0\sigma} n_{0-\sigma}\rangle\rangle$$
$$+ \langle\langle c^+_{k-\sigma} f_{0\sigma} c_{k-\sigma} | f^+_{0\sigma} n_{0-\sigma}\rangle\rangle)\,. \tag{42}$$

It is transparent that the construction of the approximations (40)–(42) are related with the small-V expansion and is not unique, but very natural. As a result we find the explicit expression for the GF in (35)

$$\langle\langle f_{0\sigma} n_{0-\sigma} | f^+_{0\sigma} n_{0-\sigma}\rangle\rangle \approx \frac{\langle n_{0-\sigma}\rangle - F^1_\sigma(\omega)}{\omega - E_{0\sigma} - U - S_1(\omega)}\,. \tag{43}$$

Here the following notations have been used

$$S_1(\omega) = S(\omega) + \sum_k |V|^2 \left(\frac{1}{\omega - \epsilon_k - E_{0\sigma} + E_{0-\sigma}} + \frac{1}{\omega + \epsilon_k - E_{0\sigma} - E_{0-\sigma} - U}\right), \tag{44}$$

$$F^1_\sigma = \sum_k (VF_2 + V^2 F_3)\,, \tag{45}$$

$$F_2 = \frac{\langle c^+_{k-\sigma} f_{0\sigma} f^+_{0\sigma} f_{0-\sigma}\rangle}{\omega + \epsilon_k - E_{0\sigma} - E_{0-\sigma} - U} + \frac{\langle f^+_{0-\sigma} c_{k-\sigma} n_{0\sigma}\rangle}{\omega - \epsilon_k - E_{0\sigma} + E_{0-\sigma}}\,, \tag{46}$$

$$F_3 = \frac{\langle\langle c_{k-\sigma} c^+_{k-\sigma} f_{0\sigma} | f^+_{0\sigma} n_{0-\sigma}\rangle\rangle}{\omega - \epsilon_k - E_{0\sigma} + E_{0-\sigma}} + \frac{\langle\langle c^+_{k-\sigma} f_{0\sigma} c_{k-\sigma} | f^+_{0\sigma} n_{0-\sigma}\rangle\rangle}{\omega + \epsilon_k - E_{0\sigma} - E_{0-\sigma} - U}\,. \tag{47}$$

Now one can substitute the GF in (35) by the expression (43). This will give to us the new approximative dynamical solution of SIAM where the complex expansion in both U and V have been incorporated. The important observation is that this new solution satisfies both limits (6). For example, if we wish to get a lowest order approximation up to U^2, V^2, it is very easy to notice that for $V = 0$:

$$\langle\langle f_{0\sigma} c^+_{k-\sigma} c_{k-\sigma} | f^+_{0\sigma} n_{0-\sigma}\rangle\rangle \approx \frac{\langle c^+_{k-\sigma} c_{k-\sigma}\rangle\langle n_{0-\sigma}\rangle}{\omega - E_{0\sigma} - U}\,,$$
$$\langle\langle c_{k-\sigma} c^+_{k-\sigma} f_{0\sigma} | f^+_{0\sigma} n_{0-\sigma}\rangle\rangle \approx \frac{\langle c_{k-\sigma} c^+_{k-\sigma}\rangle\langle n_{0-\sigma}\rangle}{\omega - E_{0\sigma} - U}\,. \tag{48}$$

This results in the possibility to find explicitly all necessary quantities and, thus, to solve the problem in a self-consistent way.

There are numerous other possibilities that lead to a more advanced and sophisticated solutions. It will be shown in separate paper that the system of equations (40)–(42) lead us to a possibility to incorporate the U-perturbation expansion (26) in our new solution for the GF (35).

7. Irreducible Green Functions Approach

After developing some of the basic facts about the correct functional structure of the relevant dynamical solution of the SIAM we are looking for, we shall give a more instructive considerations. Thus we are led to search the most suitable choice for "generalized mean fields" (GMF) and "effective shift" for SIAM. An advanced many-body method that had led to the discovery of such GMF and interpolating solutions of the Anderson/Hubbard model was proposed in Refs. 47, 5, 6 and 41. It turns out that the various solutions of the Anderson/Hubbard model are in fact given by this IGF method for various different choice of the relevant generalized mean fields. The Neal's approach remind (but not coincide with) that of the more systematic IGF method. In what follows, we shall pretend to combine the above mentioned circle of ideas in a more consistent and unified scheme.

The essense of the method of IGF is as follows. The introduction of the irreducible parts of the GFs results in separation of all suitable renormalizations of the "generalized mean fields" (GMF). As a result, without having to make any truncation of the hierarchy of equations for the GFs, one can write down a Dyson equation (in terms of retarded GFs)

$$G = G^{\mathrm{MF}} + G^{\mathrm{MF}} M G \tag{49}$$

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

$$M = (G^{\mathrm{MF}})^{-1} - G^{-1}. \tag{50}$$

Approximate solutions are constructed as definite approximations for the self-energy, in another words on the level of the higher-order GFs. It was demonstrated in Refs. 5 and 41 how to get relevant approximations for the self-energy by means of suitable approximation for high-order GF. In the present work we will use an essentially new method. We shall write an equation of motion for the higher-order GF and then, using an exact relation between initial and higher-order GFs, derive complex expansion in U and V for one-particle propagator. It is necessary to emphasize that there is an intimate connection between adequate introductions of mean fields and internal symmetries of the Hamiltonian. Though we do not want to go here into the mathematical subtleties of defining the correct mean fields for different models, we shall mention only that GMF can exhibit a quite nontrivial structure, especially for the strongly correlated case.[5,6] To obtain this structure correctly, one must construct the full GF from the complete algebra of relevant operators.

It was shown in Ref. 41, using the minimal algebra of relevant operators, that the construction of the GMFs 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.

In this paper we want to continue this line of consideration dealing with a more extended new algebra of operators from which the relevant matrix GF will be constructing. In the same spirit it belongs to the most important intentions of this work to provide the basis for future consideration of the self-consistent interpolation dynamical solutions of a few-impurity Anderson model, which will be done in separate papers elsewhere.

We now return to the IGF method again and consider how to generalize solution (3) with IGF approach in a self-consistent way. Let us consider the following equation of motion in the matrix form

$$\sum_p F(p,k)G_\sigma(p,\omega) = I + \sum_p V_p D(p,\omega) \tag{51}$$

where G is initial 4×4 matrix GF and D is the higher-order GF:

$$G_\sigma = \begin{pmatrix} G_{11} & G_{12} & G_{13} & G_{14} \\ G_{21} & G_{22} & G_{23} & G_{24} \\ G_{31} & G_{32} & G_{33} & G_{34} \\ G_{41} & G_{42} & G_{43} & G_{44} \end{pmatrix}. \tag{52}$$

Here the following notations have been used

$$\begin{aligned}
&G_{11} = \langle\langle c_{k\sigma} | c^+_{k\sigma} \rangle\rangle; && G_{12} = \langle\langle c_{k\sigma} | f^+_{0\sigma} \rangle\rangle; \\
&G_{13} = \langle\langle c_{k\sigma} | f^+_{0\sigma} n_{0-\sigma} \rangle\rangle; && G_{14} = \langle\langle c_{k\sigma} | c^+_{k\sigma} n_{0-\sigma} \rangle\rangle; \\
&G_{21} = \langle\langle f_{0\sigma} | c^+_{k\sigma} \rangle\rangle; && G_{22} = \langle\langle f_{0\sigma} | f^+_{0\sigma} \rangle\rangle; \\
&G_{23} = \langle\langle f_{0\sigma} | f^+_{0\sigma} n_{0-\sigma} \rangle\rangle; && G_{24} = \langle\langle f_{0\sigma} | c^+_{k\sigma} n_{0-\sigma} \rangle\rangle; \\
&G_{31} = \langle\langle f_{0\sigma} n_{0-\sigma} | c^+_{k\sigma} \rangle\rangle; && G_{32} = \langle\langle f_{0\sigma} n_{0-\sigma} | f^+_{0\sigma} \rangle\rangle; \\
&G_{33} = \langle\langle f_{0\sigma} n_{0-\sigma} | f^+_{0\sigma} n_{0-\sigma} \rangle\rangle; && G_{34} = \langle\langle f_{0\sigma} n_{0-\sigma} | c^+_{k\sigma} n_{0-\sigma} \rangle\rangle; \\
&G_{41} = \langle\langle c_{k\sigma} n_{0-\sigma} | c^+_{k\sigma} \rangle\rangle; && G_{42} = \langle\langle c_{k\sigma} n_{0-\sigma} | f^+_{0\sigma} \rangle\rangle; \\
&G_{43} = \langle\langle c_{k\sigma} n_{0-\sigma} | f^+_{0\sigma} n_{0-\sigma} \rangle\rangle; && G_{44} = \langle\langle c_{k\sigma} n_{0-\sigma} | c^+_{k\sigma} n_{0-\sigma} \rangle\rangle.
\end{aligned} \tag{53}$$

We avoid to write down explicitly the relevant 16 GFs from which matrix GF D consist of for the brevity. For our aims here it will be enough to proceed forth in the following way.

The equation (51) results from the first-time differentiation of the GF G and is a starting point for the IGF approach. Let us introduce the irreducible part for the higher-order GF D, by definition, in the following way (cf. Refs. 5 and 41):

$$D_\beta^{ir} = D_\beta - \sum_\alpha L^{\beta\alpha} G_{\alpha\beta}\,; \quad (\alpha,\beta) = (1,2,3,4) \tag{54}$$

and define the GMF GF according to

$$\sum_p \tilde{F}(p,k) G_\sigma^{\mathrm{MF}}(p,\omega) = I\,, \tag{55}$$

then we will be able to write down explicitly the Dyson equation (49) and the exact expression for the self-energy M (50) in the matrix form:

$$M_\sigma(k,\omega) = I^{-1} \sum_{p,q} V_p V_q \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & M_{33} & M_{34} \\ 0 & 0 & M_{43} & M_{44} \end{pmatrix} I^{-1}\,. \tag{56}$$

Here matrix I is given by

$$\begin{pmatrix} 1 & 0 & 0 & \langle n_{0-\sigma}\rangle \\ 0 & 1 & \langle n_{0-\sigma}\rangle & 0 \\ 0 & \langle n_{0-\sigma}\rangle & \langle n_{0-\sigma}\rangle & 0 \\ \langle n_{0-\sigma}\rangle & 0 & 0 & \langle n_{0-\sigma}\rangle \end{pmatrix}$$

and the matrix elements of M have the form:

$$M_{33} = \langle\langle A_1^{ir}(p) | B_1^{ir}(q)\rangle\rangle\,, \qquad M_{34} = \langle\langle A_1^{ir}(p) | B_2^{ir}(k,q)\rangle\rangle\,,$$
$$M_{43} = \langle\langle A_2^{ir}(k,p) | B_1^{ir}(q)\rangle\rangle\,, \qquad M_{44} = \langle\langle A_2^{ir}(k,p) | B_2^{ir}(k,q)\rangle\rangle\,,$$

where

$$\begin{aligned} A_1(p) &= (c_{p-\sigma}^+ f_{0\sigma} f_{0-\sigma} - c_{p-\sigma} f_{0-\sigma}^+ f_{0\sigma})\,; \\ A_2(k,p) &= (c_{k\sigma} f_{0-\sigma}^+ c_{p-\sigma} - c_{k\sigma} c_{p-\sigma}^+ f_{0-\sigma})\,; \\ B_1(p) &= (f_{0\sigma}^+ c_{p-\sigma}^+ f_{0-\sigma} - f_{0\sigma}^+ f_{0-\sigma}^+ c_{p-\sigma})\,; \\ B_2(k,p) &= (c_{k\sigma}^+ c_{p-\sigma}^+ f_{0-\sigma} - c_{k\sigma}^+ f_{0-\sigma}^+ c_{p-\sigma})\,. \end{aligned} \tag{57}$$

Since 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 the physical assumptions about this scattering.

To get an idea about the functional structure of our GMF solution (55) let us write down the matrix element G_{33}^{MF}:

$$G_{33}^{\mathrm{MF}} = \langle\langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^{+} n_{0-\sigma} \rangle\rangle$$

$$= \frac{\langle n_{0-\sigma} \rangle}{\omega - E_{0\sigma}^{\mathrm{MF}} - U - S^{\mathrm{MF}}(\omega) - Y(\omega)}$$

$$+ \frac{\langle n_{0-\sigma} \rangle Z(\omega)}{(\omega - E_{0\sigma}^{\mathrm{MF}} - U - S^{\mathrm{MF}}(\omega) - Y(\omega))(\omega - E_{0\sigma} - S(\omega))}, \tag{58}$$

$$Y(\omega) = \frac{U Z(\omega)}{\omega - E_{0\sigma} - S(\omega)}, \tag{59}$$

$$Z(\omega) = S(\omega) \sum_{p} \frac{V_P L_{41}}{\omega - \epsilon_p^{\mathrm{MF}}} + \sum_{p} \frac{|V_p|^2 L^{42}}{\omega - \epsilon_p^{\mathrm{MF}}} + S(\omega) L^{31} + \sum_{p} V_p L^{32}. \tag{60}$$

Here the coefficients L^{41}, L^{42}, L^{31} and L^{32} are the certain complicated averages (see definition (54)) from which the functional of the GMF is build. If we insert our GMF solution (58) in (35) we shall get an essentially new dynamical solution of SIAM, which is constructed on the basis of the complex (combined) expansion of the propagator in both U and V parameters and which reproduces the exact solutions of SIAM for $V = 0$ and $U = 0$. It generalizes (even on the mean-field level) the solutions of Refs. 34 and 36.

At this point it is worth to discuss some of the issues involved in deciding whether or not the solution of Ref. 8 is "exact". Let us consider the first equation of motion (51), before introducing of the irreducible GFs (54). Let us put simply in this equation the higher-order GF $D = 0$! To distinguish this simplest equation from the GMF one (55) we write it in the following form

$$\sum_{p} F(p,k) G^{0}(p,\omega) = I. \tag{61}$$

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

$$G_{22}^{0} = \langle\langle f_{0\sigma} | f_{0\sigma}^{+} \rangle\rangle = \frac{1 - \langle n_{0-\sigma} \rangle}{\omega - E_{0\sigma} - S(\omega)} + \frac{\langle n_{0-\sigma} \rangle}{\omega - E_{0\sigma} - S(\omega) - U}, \tag{62}$$

$$G_{33}^{0} = \langle\langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^{+} n_{0-\sigma} \rangle\rangle = \frac{\langle n_{0-\sigma} \rangle}{\omega - E_{0\sigma} - S(\omega) - U} \tag{63}$$

$$G_{32}^{0} = \langle\langle f_{0\sigma} n_{0-\sigma} | f_{0\sigma}^{+} \rangle\rangle = G_{33}^{0}. \tag{64}$$

The conclusion is rather evident. The results of Ref. 8 follows from our matrix GF (52) in the lowest order in V, even before introduction of GMF corrections, not

speaking about of the self-energy corrections. The two GFs G^0_{32} and G^0_{33} are equal only in the lowest order in V. It is quite clear, that the full solution

$$G^{-1} = [(G^{\mathrm{MF}})^{-1} - M] \tag{65}$$

which includes the self-energy corrections (56), is much richer.

In fact, it is very easy to rewrite the system of the equations of motion (2)–(4) of Ref. 8 in the completely equivalent form, which coincide with equation (33). As was mentioned above, identity (33) has been derived in Ref. 41. Here we used this identity in quite another way than in Ref. 41 to get the new complex expansion for the single-particle propagator. The identity (33) permit also to reformulate the problem of the derivation of the suitable interpolative solution of the SIAM, including the U-perturbation expansion, on the rather different then the single-particle GF level, on the level of the higher-order GFs as it will be shown in a separate publication.[48]

It is worthwhile to underline that our 4×4 matrix GMF GF (52) gives only approximative description of the suitable mean fields. If we shall consider more extended algebra, we shall get the more correct structure of the relevant GMF. A more rigorous mathematical derivation of this relevant algebra, showing its central importance for the self-consistent dynamical solution of SIAM, will be presented elsewhere.

8. Discussion

In summary, we presented in this paper a consistent many-body approach to analytical dynamical solution of SIAM at finite temperatures and for the broad interval of the values of the model parameters. We used an exact result (33) to connect the single-particle GF with the higher-order GF to obtain a complex combined expansion in terms of U and V for the propagator, which is similar to that of Ref. 36 but differs in a more correct identification and separation of elastic (mean fields) and inelastic (damping) contributions to the self-energy. To summarize, we therefore reformulated the problem of searches for appropriate many-body dynamical solution for SIAM in a way which provides us with an effective and workable scheme for the constructing of advanced analytical approximative solutions for the single-particle GFs on the level of the higher-order GFs in a rather systematic and a self-consistent way. This procedure has the advantage that it systematically uses the principle of interpolating solution within equation-of-motion approach for the GFs. The leading principle, which we have 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 GFs in accordance with this structure.

The main results of our IGF study are the exact Dyson equation (49) for the full 4×4 matrix GF (52) and the new derivation of the GMF GF (55). The approximative explicit calculations of the inelastic self-energy corrections are quite straightforward but tedious and too extended for the presentation here. It will be

done in the following paper soon. Here we want to emphasize the essentially new point of view on the derivation of the Generalized Mean Fields for SIAM when we are interested in the interpolating finite temperature solution for the single-particle propagator. Our final solution ((33) with (58)) has the correct functional structure and differs essentially from our previous solution in Ref. 41 where the different algebra of the relevant operators has been used.

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 left open in Refs. 36 and 34 too). 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 paper we have concentrated on the problem of correct functional structure of the single-particle GF itself. The numerical calculations will be done in separate publication elsewhere. Our main result reveals the fundamental importance of the adequate definition of the Generalized Mean Fields at finite temperatures, which results in a more deep insight into the nature of quasiparticle states of the correlated lattice fermions. We believe that our approach offers a new way for the systematic constructions of the approximative dynamical solutions of SIAM, TIAM, PAM and other models of the strongly correlated electron systems. The work in this direction is in progress.

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