Physica A 198 (1993) 606–636
North-Holland

SDI: 0378-4371(93)E0171-A

PHYSICA A

Non-local correlations and quasiparticle interactions in the Anderson model

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Received 20 April 1993

A comparative study of real many-body dynamics of single-impurity, two-impurity and periodic Anderson models (SIAM, TIAM, PAM) is performed using a recently developed irreducible Green's function method. A detailed analysis of the correct definitions of the generalized mean field corrections is given for both weak and strong Coulomb correlations. We find that for the strongly correlated regime the mean field renormalizations are described by complicated correlations which do not reduce to the functional of mean densities of electrons. The approach we suggest permits to calculate in a self-consistent way the damping of quasiparticles in both considered limits, i.e. weak and strong correlations. Also this approach gives a complete and compact description of many-body dynamics for the considered system. The corresponding spectrum consists of a broad continuous spectrum and a few localized levels embedded in the continuum. Finally we point out the implications of our results for the problem of interplay between single-site Kondo screening and interimpurity RKKY interaction.

1. Introduction

Intersite correlation effects in metal alloys and, especially, in anomalous rare-earth compounds and alloys have been the topic of growing interest recently. At low temperatures, dilute magnetic alloys show remarkable properties, which are mainly related to the single-site Kondo effect [1,2]. In ref. [1], however, it has been noticed that even in the typical dilute metal alloys there are always traces of interimpurity correlations. These interimpurity

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correlation effects can lead to suppression of Kondo behaviour, formation of clusters, etc. [3–7]. In the systems that contain rare earth ions the specific low-temperature behaviour mainly shows large conduction electron masses [8]. For the heavy fermion systems the problem of interimpurity correlations is related to the understanding of their magnetic properties [9,10].

Very recently a new development in the field has emerged which is related to alloy systems in which radical changes in physical properties occur with relatively modest changes in chemical composition [11–17]. A principle importance of these studies is connected with a fundamental problem of electronic solid state theory, namely with the tendency of 3d electrons in transition metal compounds and 4f electrons in rare-earth compounds to exhibit both localized and delocalized behaviours. The interesting electronic and magnetic properties of these substances are intimately related to this dual behaviour of electrons. In spite of experimental and theoretical achievements, still a lot remains to be understood concerning such systems. A satisfactory overall picture is still in the process of evolution.

The formation of the singlet state for the single-impurity Anderson and Kondo problem is now very well understood within the Bethe–ansatz scheme [1]. As for dynamical properties, even for the single-impurity Anderson model, the problem is only partially understood at present. The dynamics of the Anderson Hamiltonian is even more complicated than the dynamics of the Hubbard model. However, both of them are often referred to as the simplest models of magnetic metals and alloys. This naive perception contradicts the enormous amount of theoretical papers which has been published during the last decades and devoted to attacking the Anderson and Hubbard models by many refined theoretical techniques [18–22]. As is well known now [1], the simplicity of the Anderson and Hubbard models manifest itself in the dynamics of a two-particle scattering. Nevertheless as to the true many-body dynamics, there is still no simple and compact description, except in a very few limiting cases.

The inclusion of interimpurity correlations makes the problem even more difficult [23]. More recent calculations for two impurity Anderson and Kondo models [24–32] conclude that an analytical solution of the problem seems hardly possible. To attack two-impurity problems many advanced methods of quantum statistical mechanics have been used [27]. These methods, however, were not successful. The most interesting difficulty, which has been pointed out in ref. [29], is that in any order of perturbation theory, logarithmically divergent diagrams appear which cannot be generated from any divergent diagrams in a previous order. All such diagrams appear to have the feature that the Kondo effect at one site is interrupted by the spin flip between two sites induced by their mutual interaction. Another method which fails for two-

impurity problems for similar reasons is the path-integral method [29]. As to the Bethe-ansatz method, it cannot be applied in standard form. The singe-site regime is vital for one-dimensional Bethe parametrization of the spectrum in terms of the rapidities, which characterize the state of a many-body system [33].

In the present paper we propose a general theory of interimpurity correlations on the basis of different points of view [26,27] in connection with real many-body dynamics. We pay attention to the calculation of single-electron quasiparticle spectra for the two-impurity Anderson model (TIAM), treating exactly the mutual multiple elastic scattering by use of the irreducible Green's function approach [34,35]. Thus our theory for the weak Coulomb correlation case is a natural extension of the Hartree–Fock theories to include the inelastic electron–electron and electron–magnon interactions in a self-consistent way. Another important modification which has been already introduced by one of us [36] to describe the single-impurity Anderson model (SIAM) is the matrix formalism. The matrix form of the whole calculation procedure, which has never been done before, reveals many very important features and hidden difficulties of SIAM, TIAM and the cluster-impurity Anderson model (CIAM). Because these aspects of the problem are of great importance and are still not yet clarified completely, we briefly discuss these questions here. We will discuss the SIAM and TIAM, and their limitations too.

Of further interest is the problem of adequate description of many-body dynamics for the case of very strong Coulomb correlations. A number of other approaches for the strongly correlated electronic systems have been proposed, trying to find an answer to Anderson's question: "... whether a real many-body theory would give answers radically different from the Hartree–Fock (H–F) results?" [37]. By applying our theory to SIAM and TIAM we obtain an essentially new (and "radically different from the H–F") solution for the strongly correlated case. Moreover, the general concept of constructing the interpolated dynamical solution between SIAM and TIAM arises naturally in the framework of our approach. It is worthy to emphasize that the approach we suggest is founded on the same type of concept which has been proved to be valuable for various many-body systems with complicated many-branch spectra and strong interactions [34–36,38–40]. The unified concept of relevant generalized mean-field is indispensable to understand the real many-body dynamics of SIAM and TIAM. The importance of the irreducible Green's function (IGF) formalism lies in the fact that it gives a compact and convenient description of the dynamic behaviour of a system of continuous spectrum with a strongly localized perturbation (i.e., a Fermi sea of conduction electrons with a single (s-type) impurity orbital). Since the pioneering work of Friedel [41] the concept of virtual bound state (or resonant scattering state) is also indispens-

able to understand local perturbations in narrow bands of transition and rare-earth metal compounds. There are, however, several appreciable differences between Friedel's [41] and Anderson's [37] pictures which have been clarified by Blandin [42]. Namely, he clearly pointed out the essence of the whole problem: local perturbations in narrow d-bands of transition metals can be discussed within an extended Slater–Koster model. Moreover within the H–F approximation one can easily see evidence for bound state. The phase-shift analysis, taking into account the symmetry of the problem, is also particularly fruitful, but only in the single-impurity case. Outside the H–F approximation and in the many-impurity case, big problems remain open: among them, the basic problem of calculating the adequate parameters of SIAM within modern band structure theory and multi-orbital impurity states. Even for the case of SIAM this problem is quite difficult and we did not attempt to consider it, neither for SIAM nor for TIAM. However, the detailed presentation and discussion of the dynamical properties of TIAM we give here will anyway be useful to understand better the limits of applicability of the traditional models to real substances.

The present paper is divided into eight sections. In the second one the description of SIAM, TIAM and PAM is specified and a general discussion of the adequacy of those models is given. In the third section a brief outline of the IGF method is presented. In the fourth section the problem of interrelations between SIAM, TIAM, CIAM and PAM is considered. The quasiparticle spectrum of PAM is calculated within IGF approach. In section 5 the spectrum of the quasiparticle excitations and their damping is calculated for TIAM in the weakly correlated case. The role of interimpurity correlations is clearly shown. The case of very strong Coulomb correlations is considered in section 6 for SIAM. Then this approach is used in section 7 in the case of TIAM. The results of our comparative study of the differing Anderson models are discussed in the concluding section 8.

2. Presentation of the model

In the case of SIAM and by including the correlation effects in the low density case, Schrieffer and Mattis [44–45] showed that the criterion for the occurrence of magnetic moments (which has been deduced by Anderson within H–F approximation) does not hold. The solution is never magnetic. So arises the problem of the role of the electronic correlation effects [44–45]. The two-impurity Anderson model (TIAM) has been first proposed by Alexander and Anderson [43]. They have put forward a theory which introduces the impurity–impurity interaction within a game of parameters.

They assume a Hamiltonian [43]

$$H = H_{\mathrm{s}} + H_{\mathrm{d}} + H_{\mathrm{sd}} , \tag{1}$$

where

$$H_{\mathrm{s}} = \sum_{k\sigma} \varepsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} \tag{2}$$

is the Hamiltonian of a set of conduction, quasi-free electrons and the $\{\varepsilon_k\}$'s are the corresponding energies; $c^{\dagger}_{k\sigma}$ and $c_{k\sigma}$ are the creation and annihilation operators for an electron with momentum $\boldsymbol{k}$ in spin state σ,

$$H_{\mathrm{d}} = \sum_{\sigma i=1,2} E_{0i} n^{\mathrm{d}}_{i\sigma} + \frac{U}{2} \sum_{\sigma i=1,2} n^{\mathrm{d}}_{i\sigma} n^{\mathrm{d}}_{i-\sigma} + \sum_{\sigma} (V_{12} d^{\dagger}_{1\sigma} d_{2\sigma} + V_{21} d^{\dagger}_{2\sigma} d_{1\sigma}) , \tag{3}$$

where the $\{E_{0i}\}$'s are the position energies of the localized states (for simplicity we consider identical impurities and only s-type (i.e. non-degenerate) orbitals which we call d): $E_{01} = E_{02} = E_0$, U is the intraorbital Coulomb repulsion, V_{12} is the direct transfer integral between the two d states and $d^{\dagger}_{i\sigma}, d_{i\sigma}$ are, respectively, creation and annihilation operators for a d electron of spin σ at site i; $n^{\mathrm{d}}_{i\sigma}$ is the corresponding number operator. The most important term, which contains the essence of the specific behaviour of the Anderson model, is

$$H_{\mathrm{sd}} = \sum_{ik\sigma} (V_{ki} c^{\dagger}_{k\sigma} d_{i\sigma} + V_{ik} d^{\dagger}_{i\sigma} c_{k\sigma}) . \tag{4}$$

This term describes the hybridization interaction term between the localized impurity states and extended conduction states.

The definition of the hybridization matrix elements V_{ik} has been given by Anderson in his SIAM [37] as follows:

$$V_{\mathrm{dk}} = \frac{1}{\sqrt{N}} \sum_{R_n \neq 0} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_n} V_{\mathrm{d}}(\boldsymbol{R}_n) , \tag{5a}$$

with

$$V_{\mathrm{d}}(\boldsymbol{R}_n) = \int \varphi^{*}_{\mathrm{d}}(\boldsymbol{r})\, H^{\mathrm{H-F}}(\boldsymbol{r})\, a(\boldsymbol{r} - \boldsymbol{R}_n)\, \mathrm{d}\boldsymbol{r} . \tag{5b}$$

The use of $H^{\mathrm{H-F}}$ in the r.h.s. of eq. (5b) is notable, since it justifies the treatment of the SIAM entirely in the H–F approximation. As for the TIAM, the situation with the right definitions of the parameters V_{12} and V_{ik} in eqs. (3)

and (4) is rather unclear. The definition of V_{12}, as it was given in ref. [43], is the following:

$$V_{12} = V_{21}^{*} = \int \varphi_1^{*}(\boldsymbol{r})\, \varphi_2(\boldsymbol{r})\, H_{\mathrm{d}}\, \mathrm{d}\boldsymbol{r} \tag{6}$$

(now H_{d} without "H–F" mark). The essentially local character of H_{d}, eq. (3), clearly shows that V_{12} describes the direct coupling between nearest neighbouring sites. The SIAM is rather a straightforward adaptation of the Hartree–Fock picture for the wave functions to the language of the second-quantified operator representation [37],

$$d_{n\sigma}^{\dagger} = \sum_{k} \langle n|\boldsymbol{k}\rangle_{\sigma} c_{k\sigma}^{\dagger} + \langle n|d\rangle_{\sigma} d_{0\sigma}^{\dagger}\,, \tag{7}$$

where $d_{n\sigma}^{\dagger}$ is the one-electron creation operator consistent with the one-electron energy $\varepsilon_{(n)}$ which results from the relevant H–F equations. This scheme has not been analyzed in details for TIAM. The reason for that is rather evident. The justification of the TIAM needs a certain generalization of eq. (7) in the form

$$d_{n\sigma}^{\dagger} = \sum_{k} \langle n|k\rangle_{\sigma} c_{k\sigma}^{\dagger} + \langle n|d_1\rangle_{\sigma} d_{1\sigma}^{\dagger} + \langle n|d_2\rangle_{\sigma} d_{2\sigma}^{\dagger}\,. \tag{8}$$

Going back to SIAM, it has been shown that eq. (7) actually leads to omitting many interesting terms [1] like $c^{\dagger}dcd$, $c^{\dagger}c^{\dagger}dd$, etc. But the term $c^{\dagger}dcd$ just describes the contact exchange coupling which definitively must be compared to the V_{12} term for TIAM. In addition, with two new indices $i = 1, 2$, the number of omitted terms are greatly increased.

For TIAM there is a possibility of using new basis states, the so-called "even" and "odd" parity states [46,47], e.g. $d_{p\sigma} = (d_{1\sigma} \pm d_{2\sigma})/\sqrt{2}$ with p = e for even $(+1)$ and p = o for odd (-1). Then the Hamiltonian will conserve parity and can be expressed in terms of creation and annihilation operators with parity. It leads to a two parity channel problem instead of a two impurity problem [6].

Our main interest in this paper is connected with situations when the virtual-mixing mechanism is dominant and the term V_{12} plays no essential role. Also we mention only briefly the recent analysis of the applicability of the Anderson effective Hamiltonian to the 4f-phenomena in relation to photoelectron spectroscopy [48]. The claim is that the effective parameters in the Anderson Hamiltonian should be in principle frequency dependent, because the Anderson model is thought to be an effective Hamiltonian for the low

frequency phenomena. In the high frequency phenomena a more general fundamental Hamiltonian must be used. This last statement is quite interesting (compare with ref. [49]) but it needs however a separate discussion.

To summarize this chapter we conclude that, despite the well founded derivation of the TIAM, the latter could at most be considered as a reasonable semi-empirical model. Rather than attempting to calculate the parameters of the TIAM we shall give a detailed discussion of its many-body dynamics which is of particular interest. In the next sections we shall show how the self-consistent treatment of the dynamics yields a far better understanding of the SIAM and the TIAM itself.

3. Outline of the method

At this point it is worthwhile to underline that it is essential to apply an adequate method in order to solve a concrete physical problem: the final solution should contain a correct physical reasoning in a most natural way. The list of many-body techniques that have been applied to the Anderson model is extensive [1,2,18–32]. In this paper it will be attempted to justify the use of a novel IGF approach [34–36] to SIAM and TIAM. It is quite revealing to follow the logic of development of many-body techniques. This logic is well known. The simple Hartree–Fock or RPA treatment of the correlations between electrons omits several essential features. One of them is the damping of quasiparticles. Usually, this latter problem requires much larger theoretical efforts. However, this must be a final goal towards a real understanding of many-body dynamics in strongly correlated electronic systems.

The IGF method allows one to describe completely the quasiparticle spectra with damping in a very general way. It is based on the notion of the "irreducible" parts of the GF's (or the irreducible parts of the operators, out of which the GF's are built). In terms of the IGF's it is then possible, without recourse to a truncation of the hierarchy of equations, to write down the exact Dyson equation and to obtain an exact analytical representation of the self-energy operator. Therefore, in contrast to the standard equation-of-motion approach, the decoupling is introduced in the self-energy operator only. The general philosophy of the IGF method lies in the separation and identification of elastic scattering effects and inelastic ones. This last point is quite often underestimated, since there are quite a lot of works where both effects are mixed. However, as far as the right definition of quasiparticle damping is concerned, the separation of elastic and inelastic scattering process is believed to be crucially important for the many-body systems with complicated many-branch spectrum and strong interactions [34–36,38–40].

The IGF's are defined in such a way that they cannot be reduced to the lower-order ones by any way of decoupling. This procedure extracts all relevant (for the problem under consideration) mean-field contributions (elastic scattering terms) and puts them into the generalized mean-field GF's. It is worth emphasizing that, in general, the mean-field renormalizations can exhibit a quite nontrivial structure. To obtain this structure correctly, one must construct the full GF's from the complete algebra of relevant operators and develop a special projection procedure for higher-order GF's in accordance with a given algebra.

4. The hierarchy of the Anderson models

It will be quite revealing to discuss the interrelations of SIAM, TIAM and PAM (as well as a cluster impurity periodic Anderson model (CIPAM), which has been described in details by ref. [50]). The basic assumption of the periodic impurity Anderson model approach is the presence of two very well defined subsystems, i.e. the Fermi sea of nearly free conduction electrons and the localized impurity orbitals embedded into the preceding continuum (in rare-earth compounds for example the continuum is actually a mixture of s, p, and d states and the localized orbitals are f states). The simplest form of PAM,

$$H = \sum_{k\sigma} \varepsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{i\sigma} E_0 n^{\mathrm{d}}_{i\sigma} + \frac{U}{2} \sum_{i\sigma} n^{\mathrm{d}}_{i\sigma} n^{\mathrm{d}}_{i-\sigma} + \frac{V}{\sqrt{N}} \sum_{ik\sigma} (\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i} d^{\dagger}_{i\sigma} c_{k\sigma} + \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i} c^{\dagger}_{k\sigma} d_{i\sigma}) , \tag{9}$$

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

$$c^{\dagger}_{\boldsymbol{k}\sigma} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} c^{\dagger}_{j\sigma} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_j} , \qquad c_{k\sigma} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} c_{j\sigma} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_j} , \tag{10}$$

the Hamiltonian (9) can be rewritten in Wannier representation in the form

$$H = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i\sigma} E_0 n^{\mathrm{d}}_{i\sigma} + \frac{U}{2} \sum_{i\sigma} n^{\mathrm{d}}_{i\sigma} n^{\mathrm{d}}_{i-\sigma} + V \sum_{i\sigma} (d^{\dagger}_{i\sigma} c_{i\sigma} + c^{\dagger}_{i\sigma} d_{i\sigma}) . \tag{11}$$

If one retains the k-dependence of the hybridization matrix element V_k in eq. (11) the last term of the r.h.s. in eq. (11) will be as follows:

$$\sum_{ij\sigma} V_{ij} (d^{\dagger}_{i\sigma} c_{i\sigma} + c^{\dagger}_{i\sigma} d_{j\sigma}) , \qquad V_{ij} = \frac{1}{N} \sum_{k} V_k \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}_j - \boldsymbol{R}_i)} . \tag{12}$$

The on-site hybridization V_{ii} is equal to zero for symmetry reasons. Moreover as compared to the SIAM, the PAM has its own specific features. This can lead to peculiar magnetic properties for concentrated rare earth systems [50] where the criterion for magnetic ordering depends on the competition between indirect RKKY-type interaction (not included in SIAM) and the Kondo-type singlet state screening (contained in SIAM). Instead of carrying through such a laborious programme in the rare earth systems for example, we will consider here a simpler case, namely the comparison of the dynamical behaviours of SIAM and PAM in the limit of weak Coulomb correlations. Of course, this is not directly related to Kondo-type behaviours which show up in the strongly correlated ($U \to \infty$) regime [51]. However, this comparison procedure will be very instructive for future analysis of TIAM. Let us consider the PAM in Bloch representation,

$$H = \sum_{k\sigma} \varepsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{k\sigma} E(k)\, d^{\dagger}_{k\sigma} d_{k\sigma} + \frac{U}{2N} \sum_{pqr\sigma} d^{\dagger}_{p+r-q,\sigma} d_{p\sigma} d^{\dagger}_{q,-\sigma} d_{r,-\sigma} + \sum_{k\sigma} V_k (d^{\dagger}_{k\sigma} c_{k\sigma} + c^{\dagger}_{k\sigma} d_{k\sigma}) \,. \tag{13}$$

For simplicity in this section we will discuss the case when $U \to 0$. The more basic drawback of the Hartree–Fock type solution is that it ignores the correlation of the "up" and "down" electrons. Actually we will take into account the latter correlation for the PAM and SIAM in a self-consistent way using the IGF method. It can be shown that the use of the matrix Green's function for PAM,

$$\hat{G}_{k\sigma}(\omega) = \begin{bmatrix} \langle\langle c_{k\sigma} | c^{\dagger}_{k\sigma} \rangle\rangle & \langle\langle c_{k\sigma} | d^{\dagger}_{k\sigma} \rangle\rangle \\ \langle\langle d_{k\sigma} | c^{\dagger}_{k\sigma} \rangle\rangle & \langle\langle d_{k\sigma} | d^{\dagger}_{k\sigma} \rangle\rangle \end{bmatrix}, \tag{14}$$

permits to handle the relevant equations within a very compact form. The first-time d/dt equation of motion for the double-time thermal GF [52],

$$\langle\langle A(t)\, B(t') \rangle\rangle = \mathrm{i}\theta(t - t') \langle [A(t), B(t)]_{+} \rangle \,, \tag{15}$$

reads

$$\begin{bmatrix} \omega - \varepsilon_k & -V_k \\ -V_k & \omega - E(k) \end{bmatrix} \times \begin{bmatrix} \langle\langle c_{k\sigma} | c^{\dagger}_{k\sigma} \rangle\rangle_{\omega} & \langle\langle c_{k\sigma} | d^{\dagger}_{k\sigma} \rangle\rangle_{\omega} \\ \langle\langle d_{k\sigma} | c^{\dagger}_{k\sigma} \rangle\rangle_{\omega} & \langle\langle d_{k\sigma} | d^{\dagger}_{k\sigma} \rangle\rangle_{\omega} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + UN^{-1} \sum_{pq} \begin{bmatrix} 0 & 0 \\ \langle\langle A | c^{\dagger}_{k\sigma} \rangle\rangle & \langle\langle A | d^{\dagger}_{i\sigma} \rangle\rangle \end{bmatrix}, \tag{16}$$

where $A = d_{k+p,\sigma} d^{\dagger}_{p+q,-\sigma} d_{q,-\sigma}$.

According to refs. [34–36] the definition of the irreducible parts for $U \to 0$ is as follows:

$$^{\mathrm{ir}}\langle\langle d_{k+p,\sigma} d^{\dagger}_{p+q,-\sigma} d_{q,-\sigma} | c^{\dagger}_{k\sigma} \rangle\rangle = \langle\langle d_{k+p,\sigma} d^{\dagger}_{p+q,-\sigma} d_{q\sigma} | c^{\dagger}_{k\sigma} \rangle\rangle - \delta_{p,0} \langle n_{q,-\sigma} \rangle \langle\langle d_{k\sigma} | c^{\dagger}_{k\sigma} \rangle\rangle , \tag{17}$$

$$^{\mathrm{ir}}\langle\langle d_{k+p,\sigma} d^{\dagger}_{p+q,-\sigma} d_{q,-\sigma} | d^{\dagger}_{k\sigma} \rangle\rangle = \langle\langle d_{k+p,\sigma} d^{\dagger}_{p+q,-\sigma} d_{q\sigma} | d^{\dagger}_{k\sigma} \rangle\rangle - \delta_{p,0} \langle n_{q,-\sigma} \rangle \langle\langle d_{k\sigma} | d^{\dagger}_{k\sigma} \rangle\rangle , \tag{18}$$

Then we obtain after using eqs. (17, 18) in the r.h.s. of eq. (16)

$$\begin{bmatrix} \omega - \varepsilon_k & -V_k \\ -V_k & \omega - E_\sigma(k) \end{bmatrix} \begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + UN^{-1} \sum_{pq} \begin{bmatrix} 0 & 0 \\ {}^{\mathrm{ir}}\langle\langle A | c^{\dagger}_{k\sigma} \rangle\rangle_\omega & {}^{\mathrm{ir}}\langle\langle A | d^{\dagger}_{k\sigma} \rangle\rangle_\omega \end{bmatrix} . \tag{19}$$

The following notations have been used:

$$E_\sigma(k) = E(k) - U n^{\mathrm{d}}_{-\sigma} , \qquad n^{\mathrm{d}}_{-\sigma} = \langle n^{\mathrm{d}}_{k-\sigma} \rangle .$$

The definition of the generalized mean field (GMF) (which for the weakly correlated case coincides with the Hartree–Fock mean field) Green's function (GF) is evident. All inelastic renormalization terms are now related to the last term in the r.h.s. of eq. (19). All elastic scattering (or mean field) renormalization terms are contained in the following matrix equation for GMF–GF:

$$\begin{bmatrix} \omega - \varepsilon_k & -V_k \\ -V_k & \omega - E_\sigma(k) \end{bmatrix} \times \begin{bmatrix} G^0_{11} & G^0_{12} \\ G^0_{21} & G^0_{22} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} . \tag{20}$$

It is easy to solve eq. (20) and we find

$$\langle\langle d_{k\sigma} | d^{\dagger}_{k\sigma} \rangle\rangle^0_\omega = \left\{ \omega - E_\sigma(k) - \frac{|V_k|^2}{\omega - \varepsilon_k} \right\}^{-1} , \tag{21}$$

$$\langle\langle c_{k\sigma} | c^{\dagger}_{k\sigma} \rangle\rangle^0_\omega = \left\{ \omega - \varepsilon_k - \frac{|V_k|^2}{\omega - E_\sigma(k)} \right\}^{-1} . \tag{22}$$

At this point it is worthwhile to underline the significant difference between

PAM and SIAM, which was shortly mentioned in ref. [36]. The corresponding SIAM equation for GMF–GF reads [36]

$$\sum_{p}\begin{bmatrix}(\omega-\varepsilon_p)\delta_{pk} & -V_p\delta_{pk}\\ -V_p & \frac{1}{N}(\omega-E_0)\end{bmatrix}\begin{bmatrix}\langle\langle c_{p\sigma}|c^{\dagger}_{k\sigma}\rangle\rangle^{0} & \langle\langle c_{p\sigma}|d^{\dagger}_{0\sigma}\rangle\rangle^{0}\\ \langle\langle d_{0\sigma}|c^{\dagger}_{k\sigma}\rangle\rangle^{0} & \langle\langle d_{0\sigma}|d^{\dagger}_{0\sigma}\rangle\rangle^{0}\end{bmatrix}=\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}. \tag{23}$$

This form of matrix notation for SIAM has never been used before. However, it clearly shows which fundamental problem has been posed by Anderson in his famous paper [37], i.e. how to define the quasiparticle spectrum of a system with strongly localized levels embedded in a continuum of states. Within our matrix representation, the eigenvalue problem reveals a fundamental difficulty: the number of states in the conduction band and in the localized orbital are different, namely if we include the spin degeneracy the conduction band contains $2N$ states whereas the localized (s-type) level contains only 2. The comparison of eqs. (20) and (23) shows clearly that this difficulty does not exist for PAM: the number of states in both localized and delocalized subbands are the same, i.e. $2N$ (see fig. 1). There are many other relevant questions connected with the comparison between PAM and SIAM, but we believe that in order to understand the nature of the spectrum of elementary excitations this is the most fundamental one.

The eq. (23) for GMF–GF of SIAM is exactly solvable as well as the corresponding eq. (20) for PAM. However, the presence of Σ_p in eq. (23) clearly means that this solution is simply to solve for any fixed momentum p. In general, the compact solutions found by Anderson [37] are written in the following forms:

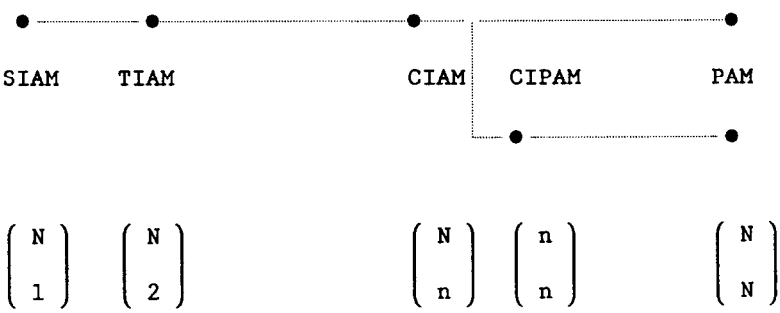

Fig. 1. The hierarchy of the Anderson models (the numbers are given in the case of 's' orbitals with $n \leqslant N$; the upper row gives the number of *conduction* states per spin and the lower row gives the number of *localized* states per spin). For a detailed presentation of the CIPAM, see also ref. [65].

$$\langle\langle d_{0\sigma}|d_{0\sigma}^{\dagger}\rangle\rangle_{\omega}^{0}=\left(\omega-E_{0\sigma}-\sum_{k}\frac{|V_k|^2}{\omega-\varepsilon_k}\right)^{-1},$$

$$\langle\langle c_{k\sigma}|c_{k\sigma}^{\dagger}\rangle\rangle_{\omega}^{0}=\frac{1}{\omega-\varepsilon_k}+\frac{|V_k|^2}{(\omega-\varepsilon_k)^2}G_{\mathrm{dd}}(\omega)\,. \tag{24}$$

The fundamental difference between SIAM and PAM plays a very essential role when we proceed with incorporating the correlation effects, i.e. when we include the inelastic scattering or self-energy corrections.

Let us again consider the PAM, starting from eq. (16). After second time differentiation $\mathrm{d}/\mathrm{d}t$ of the higher-order GF in the r.h.s. of eq. (16) and introducing irreducible parts for the r.h.s operators by analogy with eqs. (17), (18), the equation of motion (16) can be exactly rewritten in the form of the Dyson equation,

$$\hat{G}=\hat{G}^{0}+\hat{G}^{0}\hat{M}\hat{G}\,. \tag{25}$$

Note that no decoupling has been done till now but only identical transformation. The formal solution of the Dyson equation can be cast as follows:

$$\hat{G}=[(\hat{G}^{0})^{-1}-\hat{M}]^{-1}, \tag{26}$$

where the self-energy operator $\hat{M}$ has the form

$$\hat{M}_{k\sigma}(\omega)=\begin{bmatrix}0 & 0\\ 0 & M_{22}\end{bmatrix}, \tag{27}$$

with

$$\hat{M}_{22}=\frac{U^2}{N^2}\sum_{pqrs}{}^{\mathrm{ir}}\langle\langle d_{k+p,\sigma}d_{p+q,-\sigma}^{\dagger}d_{q,-\sigma}|d_{r,-\sigma}^{\dagger}d_{r+s,-\sigma}d_{k+s,\sigma}^{\dagger}\rangle\rangle_{\omega}^{\mathrm{ir}}\,. \tag{28}$$

In order to calculate the self-energy operator in a self-consistent way, we have to express it approximately by lower order GF's. However, the advantage of using the Dyson equation consists in the right functional structure of the single-particle GF. In analogy with low density electron gas we calculate the self-energy operator (28) in the pair approximation. With the help of the spectral theorem [52] we express the GF by the correlation function. Then for the correlation function we use the following so-called "trial solution" in the case of a low density of quasiparticles $\langle n\rangle \ll 1$:

$$\langle a^{\dagger}_{r,-\sigma}a_{r+s,-\sigma}a^{\dagger}_{k+s,\sigma}a_{k+p,\sigma}(t)\, a_{p+q,-\sigma}(t)\, a_{q,-\sigma}(t)\rangle^{\mathrm{ir}} \approx \langle a^{\dagger}_{k+p,\sigma}a_{k+p,\sigma}(t)\rangle$$
$$\langle a_{p+q,-\sigma}a^{\dagger}_{p+q,-\sigma}(t)\rangle\langle a^{\dagger}_{q,-\sigma}a_{q,-\sigma}(t)\rangle\delta_{k+s,k+p}\delta_{r+s,p+q}\delta_{r,q}\,. \tag{29}$$

After the substitution of eq. (29) into eq. (28) we find for the self-energy

$$M_{k\sigma}(\omega) = \frac{U^2}{N^2}\sum_{pq}\int \frac{\mathrm{d}\omega_1\,\mathrm{d}\omega_2\,\mathrm{d}\omega_3}{\omega+\omega_1-\omega_2-\omega_3}\{n(\omega_1)\,[1-n(\omega_2)-n(\omega_3)] + n(\omega_2)\,n(\omega_3)\}\, g_{p+q,-\sigma}(\omega_1)\; g_{k+p,\sigma}(\omega_2)\; g_{q,-\sigma}(\omega_3)\,, \tag{30}$$

where

$$g_{k\sigma}(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\, G_{k\sigma}(\omega+\mathrm{i}0) \tag{31}$$

is the spectral density. The eq. (30) with eq. (26) form together the self-consistent system of equations to calculate single-electron GF's and the corresponding density of states,

$$D(\omega) = \frac{1}{\pi N}\sum_{k\sigma}\mathrm{Im}\, G_{k\sigma}(\omega+\mathrm{i}0)\,. \tag{32}$$

If we start the iteration procedure with the simplest first iteration expression

$$g_{k\sigma} \sim \delta(\omega - E_{\sigma}(k))\,, \tag{33}$$

then after integration we find the standard second-order expression for the self-energy (cf. ref. [34]),

$$M_{k\sigma}(\omega) = \frac{U^2}{N^2}\sum_{pq}\frac{n_{p+q,-\sigma}(1-n_{k+p,\sigma}-n_{q,-\sigma})+n_{k+p,\sigma}n_{q,-\sigma}}{\omega+E_{\sigma}(p+q)-E_{\sigma}(k+p)-E_{\sigma}(q)}\,. \tag{34}$$

Here $n_{k\sigma} = [\exp(\beta E_{k\sigma})+1]^{-1}$ is the Fermi distribution function. It is interesting to note that the same sort of calculation for the self-energy can be done in the case of SIAM [36]. But then the pair approximation in eq. (29) does not work. Actually the analogous expression for SIAM self-energy is

$$M^{\sigma}_{00}(\omega) \approx U^2\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega_1\,\mathrm{d}\omega_2\,\mathrm{d}\omega_3}{\omega+\omega_1-\omega_2-\omega_3}\{n(\omega_1)\,[1-n(\omega_2)-n(\omega_3)] + n(\omega_2)\,n(\omega_3)\}\, g_{0-\sigma}(\omega_1)\; g_{0\sigma}(\omega_2)\; g_{0-\sigma}(\omega_3)\,, \tag{35}$$

where

$$g_{0\sigma}(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\langle\langle d_{0\sigma}|d_{0\sigma}^{\dagger}\rangle\rangle_{\omega+\mathrm{i}0} \tag{36}$$

and the first iteration expression has the form

$$g_{0\sigma}(\omega) \sim \delta(\omega - E_0 - Un_{-\sigma})\,, \tag{37}$$

then we immediately obtain $M_{00}^{\sigma} = 0$. This result reflects the fact that only one impurity site is present. The recipe to calculate the self-energy operator for SIAM has been given by ref. [36]. We will use it for TIAM in the next section 5. In the case of PAM the same kind of approximation as in ref. [36] will lead to the expression for the self-energy in the following form:

$$M_{k\sigma}(\omega) = \frac{U^2}{N}\sum_{q}\int \mathrm{d}\omega_1 \left[\coth\left(\frac{\omega-\omega_1}{2T}\right) + \tanh\left(\frac{\omega_1}{2T}\right)\right] \times \left(-\frac{1}{\pi}\,\mathrm{Im}\,\chi_q^{\mp\pm}(\omega-\omega_1)\right) g_{k+q,\sigma}(\omega_1)\,. \tag{38}$$

To conclude this section we propose in fig. 1 a possible hierarchy of the various Anderson models. Except the specific case of the SIAM we always have the situation which corresponds to inter-impurity interactions. The corresponding physical behaviour can then be understood looking through the SIAM–TIAM and CIPAM–PAM complementary solutions.

5. TIAM. Weak correlation

We again consider the TIAM Hamiltonian (1). The IGF solution of this model is obtained by analogy with the SIAM for small U.

Taking into account the first time differentiation of the relevant GF matrix, we have

$$\sum_{p}\left[\begin{array}{ccc} (\omega-\varepsilon_p)\delta_{pk} & -V_{1p}\delta_{pk} & -V_{2p}\delta_{pk} \\ -V_{1p} & \frac{1}{N}(\omega-E_0) & -V_{12} \\ -V_{2p} & -V_{21} & \frac{1}{N}(\omega-E_0) \end{array}\right] \times \left[\begin{array}{ccc} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{array}\right]$$
$$= \left[\begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array}\right] + U\left[\begin{array}{ccc} 0 & 0 & 0 \\ \langle\langle A_1|c_{k\sigma}^{\dagger}\rangle\rangle & \langle\langle A_1|d_{1\sigma}^{\dagger}\rangle\rangle & \langle\langle A_1|d_{2\sigma}^{\dagger}\rangle\rangle \\ \langle\langle A_2|c_{k\sigma}^{\dagger}\rangle\rangle & \langle\langle A_2|d_{1\sigma}^{\dagger}\rangle\rangle & \langle\langle A_2|d_{2\sigma}^{\dagger}\rangle\rangle \end{array}\right]. \tag{39}$$

The notations are as follows:

$$
\begin{aligned}
&G_{11} = \langle\langle c_{p\sigma} | c^{\dagger}_{k\sigma} \rangle\rangle , \quad && G_{12} = \langle\langle c_{p\sigma} | d^{\dagger}_{1\sigma} \rangle\rangle , \quad && G_{13} = \langle\langle c_{p\sigma} | d^{\dagger}_{2\sigma} \rangle\rangle , \\
&G_{21} = \langle\langle d_{1\sigma} | c^{\dagger}_{k\sigma} \rangle\rangle , \quad && G_{22} = \langle\langle d_{1\sigma} | d^{\dagger}_{1\sigma} \rangle\rangle , \quad && G_{23} = \langle\langle d_{1\sigma} | d^{\dagger}_{2\sigma} \rangle\rangle , \\
&G_{31} = \langle\langle d_{2\sigma} | c^{\dagger}_{k\sigma} \rangle\rangle , \quad && G_{32} = \langle\langle d_{2\sigma} | d^{\dagger}_{1\sigma} \rangle\rangle , \quad && G_{33} + \langle\langle d_{2\sigma} | d^{\dagger}_{2\sigma} \rangle\rangle , \\
&A_1 = d_{1\sigma} n_{1-\sigma} , \quad && A_2 = d_{2\sigma} n_{2-\sigma} .
\end{aligned}
\tag{40}
$$

In compact form the eq. (39) can then be expressed as

$$
\sum_p \hat{L}_{pk} \hat{G}_{pk}(\omega) = \hat{I} + U \hat{D}_k(\omega) . \tag{41}
$$

We thus have the equation of motion (39) which is a complete analog of the corresponding equations for the SIAM and PAM. Let us again introduce by definition the irreducible part of the GF's

$$
\begin{aligned}
&{}^{\mathrm{ir}}\langle\langle d_{1\sigma} n_{1-\sigma} | B \rangle\rangle = \langle\langle d_{1\sigma} n_{1-\sigma} | B \rangle\rangle - \langle n_{1-\sigma} \rangle \langle\langle d_{1\sigma} | B \rangle\rangle , \\
&{}^{\mathrm{ir}}\langle\langle d_{2\sigma} n_{2-\sigma} | B \rangle\rangle = \langle\langle d_{2\sigma} n_{2-\sigma} | B \rangle\rangle - \langle n_{2-\sigma} \rangle \langle\langle d_{2\sigma} | B \rangle\rangle ,
\end{aligned}
\tag{42}
$$

where we expect the thermal average $\langle n_{i-\sigma} \rangle$ to be uniform (in principle it is possible to consider a non-uniform solution),

$$
\langle n_{1-\sigma} \rangle = \langle n_{2-\sigma} \rangle = \langle n_{-\sigma} \rangle . \tag{43}
$$

Now, if we consider the eq. (39), taking into account the definition (42), we obtain in analogy with eq. (19) the same equation as (41); only, instead of $\hat{D}_k(\omega)$ it will contain $\hat{D}^{\mathrm{ir}}_k(\omega)$. Let us define as previously the GMF–GF in the following way:

$$
\sum_p \hat{L}_{pk} \hat{G}^0_{pk} = \hat{I} . \tag{44}
$$

After performing the second time variable differentiation in the r.h.s. of (39) and introducing the relevant irreducible parts for the GF's we are able to rewrite the equation of motion in the form of a Dyson equation

$$
\hat{G} = \hat{G}^0 + \hat{G}^0 \hat{M} \hat{G} . \tag{45}
$$

Let us remind again that $\hat{G}^0$ is defined as follows:

$$\sum_p \begin{bmatrix} (\omega - \varepsilon_p)\delta_{pk} & -V_{1p}\delta_{pk} & \vdots & -V_{2p}\delta_{pk} \\ -V_{1p} & \frac{1}{N}(\omega - E_{0\sigma}) & \vdots & -V_{12} \\ \cdots\cdots & \cdots\cdots & \vdots & \cdots\cdots \\ -V_{2p} & -V_{21} & \vdots & \frac{1}{N}(\omega - E_{0\sigma}) \end{bmatrix} \times \begin{bmatrix} G^0_{11} & G^0_{12} & \vdots & G^0_{13} \\ G^0_{21} & G^0_{22} & \vdots & G^0_{23} \\ \cdots & \cdots & \vdots & \cdots \\ G^0_{31} & G^0_{32} & \vdots & G^0_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & \vdots & 0 \\ 0 & 1 & \vdots & 0 \\ \cdots & \cdots & \vdots & \cdots \\ 0 & 0 & \vdots & 1 \end{bmatrix}. \tag{46}$$

The matrix $\hat{G}^0$ describes the exact solution of the TIAM in the H–F approximation. The SIAM–GF's are shown in the left upper corner of each matrix. We thus have a very clear representation of the essence of the nonlocal interimpurity correlation problem in the case of two localized levels interacting with a continuous spectrum of conduction electrons. The eq. (46) represents the exact solution for the considered problem in the H–F approximation. After some algebra we find the following for the diagonal elements:

$$\begin{aligned} \langle\langle c_{k\sigma} | c^\dagger_{k\sigma} \rangle\rangle^0_\omega &= \left(\omega - \varepsilon_k - \frac{|V_{1k}|^2}{\omega - E_{0\sigma}} - \Delta_{11}(k, \omega)\right)^{-1}, \\ \langle\langle d_{1\sigma} | d^\dagger_{1\sigma} \rangle\rangle^0_\omega &= \left(\omega - E_{0\sigma} - \sum_p \frac{|V_{1k}|^2}{\omega - \varepsilon_p} - \Delta_{22}(\omega)\right)^{-1}, \\ \langle\langle d_{2\sigma} | d^\dagger_{2\sigma} \rangle\rangle^0_\omega &= \left(\omega - E_{0\sigma} - \sum_p \frac{|V_{2k}|^2}{\omega - \varepsilon_p} - \Delta_{33}(\omega)\right)^{-1}. \end{aligned} \tag{47}$$

Here we have introduced the notations

$$\Delta_{11}(k, \omega) = \left(V_{2k} + \frac{V_{1k}V_{12}}{\omega - E_{0\sigma}}\right)\left(V_{2k} + \frac{V_{1k}V_{21}}{\omega - E_{0\sigma}}\right)\left(\omega - E_{0\sigma} - \frac{V_{21}V_{12}}{\omega - E_{0\sigma}}\right)^{-1}, \tag{48}$$

$$\Delta_{22}(\omega) = (\lambda_{21}(\omega) + V_{12})(\lambda_{21}(\omega) + V_{21})\left(\omega - E_{0\sigma} - \sum_p \frac{|V_{2p}|^2}{\omega - \varepsilon_p}\right)^{-1}, \tag{49}$$

$$\Delta_{33}(\omega) = (\lambda_{12}(\omega) + V_{21})(\lambda_{12}(\omega) + V_{12})\left(\omega - E_{0\sigma} - \sum_p \frac{|V_{1p}|^2}{\omega - \varepsilon_p}\right)^{-1}, \tag{50}$$

where

$$\lambda_{21}(\omega) = \lambda_{12}(\omega) = \sum_p \frac{V_{1p}V_{2p}}{\omega - \varepsilon_p} \tag{51}$$

describes the so-called "indirect coupling" [43]. If we put $V_{12} = V_{21} = 0$, we obtain

$$\Delta_{22}(\omega) = \frac{(\lambda_{12}(\omega))^2}{\omega - E_{0\sigma} - \Sigma_p |V_{2p}|^2/(\omega - \varepsilon_p)}, \tag{52}$$

$$\Delta_{33}(\omega) = \frac{(\lambda_{12}(\omega))^2}{\omega - E_{0\sigma} - \Sigma_p |V_{1p}|^2/(\omega - \varepsilon_p)}, \tag{53}$$

$$\Delta_{11}(k, \omega) = \frac{|V_{2k}|^2}{(\omega - E_{0\sigma})}. \tag{54}$$

The detailed analysis of the H–F solution for two impurities has been done previously [43, 53]. Here we will consider the quasiparticle interactions by using the Dyson equation for the TIAM.

The formal solution of the matrix Dyson, eq. (45), has the form

$$\hat{G} = [(\hat{G}^0)^{-1} - \hat{M}]^{-1}. \tag{55}$$

Let us consider the explicit expression for the self-energy matrix

$$\hat{M} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & M_{22} & M_{23} \\ 0 & M_{32} & M_{33} \end{bmatrix}, \tag{56}$$

where

$$M_{22} = U^{2\,\mathrm{ir}} \langle\langle d_{1\sigma} n_{1-\sigma} | d^\dagger_{1\sigma} n_{1-\sigma} \rangle\rangle^{\mathrm{ir}}, \qquad M_{32} = U^{2\,\mathrm{ir}} \langle\langle d_{2\sigma} n_{2-\sigma} | n_{1-\sigma} d^\dagger_{1\sigma} \rangle\rangle^{\mathrm{ir}},$$
$$M_{23} = U^{2\,\mathrm{ir}} \langle\langle d_{1\sigma} n_{1-\sigma} | n_{2-\sigma} d^\dagger_{2\sigma} \rangle\rangle^{\mathrm{ir}}, \qquad M_{33} = U^{2\,\mathrm{ir}} \langle\langle d_{2\sigma} n_{2-\sigma} | n_{2-\sigma} d^\dagger_{2\sigma} \rangle\rangle^{\mathrm{ir}}. \tag{57}$$

In order to calculate the self-energy matrix elements [57], let us perform for the TIAM the same type of procedure as it has been done previously for the SIAM [36]. With the help of the spectral theorem one can express the GF's (57) in terms of correlation functions. The natural "trial solution" for the correlation functions can be proposed in the following way [34]:

$$\langle d^{\dagger}_{1\sigma} d^{\dagger}_{1-\sigma} d_{1-\sigma} d_{1\sigma}(t)\, d^{\dagger}_{1-\sigma}(t)\, d_{1-\sigma}(t)\rangle$$
$$\approx \langle d^{\dagger}_{1-\sigma} d_{1-\sigma} d^{\dagger}_{1-\sigma}(t)\, d_{1-\sigma}(t)\rangle \langle d^{\dagger}_{1\sigma} d_{1\sigma}(t)\rangle$$
$$+ \langle d^{\dagger}_{1-\sigma} d_{1-\sigma}(t)\rangle \langle d^{\dagger}_{1\sigma} d_{1-\sigma} d_{1\sigma}(t)\, d^{\dagger}_{1-\sigma}(t)\rangle$$
$$+ \langle d_{1-\sigma} d^{\dagger}_{1-\sigma}(t)\rangle \langle d^{\dagger}_{1\sigma} d^{\dagger}_{1-\sigma} d_{1\sigma}(t)\, d_{1-\sigma}(t)\,, \tag{58}$$

$$\langle d^{\dagger}_{2\sigma} d^{\dagger}_{2-\sigma} d_{2-\sigma} d_{1\sigma}(t)\, d^{\dagger}_{1-\sigma}(t)\, d_{1-\sigma}(t)\rangle$$
$$\approx \langle d^{\dagger}_{2-\sigma} d_{2-\sigma} d^{\dagger}_{1-\sigma}(t)\, d_{1-\sigma}(t)\rangle \langle d^{\dagger}_{2\sigma} d_{1\sigma}(t)\rangle$$
$$+ \langle d^{\dagger}_{2-\sigma} d_{1-\sigma}(t)\rangle \langle d^{\dagger}_{2\sigma} d_{2-\sigma} d_{1\sigma}(t)\, d^{\dagger}_{1-\sigma}(t)\rangle$$
$$+ \langle d_{2-\sigma} d^{\dagger}_{1-\sigma}(t)\rangle \langle d^{\dagger}_{2\sigma} d^{\dagger}_{2-\sigma} d_{1\sigma}(t)\, d_{1-\sigma}(t)\rangle\,. \tag{59}$$

The terms which describe the correlations of the "up" and "down" spins on the same and different sites correspond to the second terms in the r.h.s. of eqs. (58) and (59),

$$\sum_{\sigma} \langle d^{\dagger}_{1-\sigma} d_{1-\sigma}(t)\rangle \langle d^{\dagger}_{1\sigma} d_{1-\sigma} d_{1\sigma}(t)\, d^{\dagger}_{1-\sigma}(t)\rangle$$
$$= \langle S^{\dagger}_1 S^{-}_1(t)\rangle \langle d^{\dagger}_{1\downarrow} d_{1\downarrow}\rangle + \langle S^{-}_1 S^{\dagger}_1(t)\rangle \langle d^{\dagger}_{1\uparrow} d_{1\uparrow}\rangle\,, \tag{60}$$

$$\sum_{\sigma} \langle d^{\dagger}_{2-\sigma} d_{1-\sigma}\rangle \langle d^{\dagger}_{2\sigma} d_{2-\sigma} d_{1\sigma}(t)\, d^{\dagger}_{1-\sigma}(t)\rangle$$
$$= \langle S^{\dagger}_2 S^{-}_1(t)\rangle \langle d^{\dagger}_{2\downarrow} d_{1\downarrow}\rangle + \langle S^{-}_2 S^{\dagger}_1(t)\rangle \langle d^{\dagger}_{2\uparrow} d_{1\uparrow}\rangle\,. \tag{61}$$

Here $S^{\dagger} = d^{\dagger}_{\uparrow} d_{\downarrow}$, $S^{-} = d^{\dagger}_{\downarrow} d_{\uparrow}$.

Using eqs. (58)–(61) we find the following explicit expressions for the self-energy matrix elements:

$$M^{22}_{\uparrow}(\omega) = U^2 \int_{\infty}^{\infty} \mathrm{d}\omega_1\, \mathrm{d}\omega_2 \frac{1 + N(\omega_1) - n(\omega_2)}{\omega - \omega_1 - \omega_2}$$
$$\times \left(-\frac{1}{\pi} \operatorname{Im} \langle\langle S^{-}_1 | S^{\dagger}_1 \rangle\rangle_{\omega_1}\right)\left(-\frac{1}{\pi} \operatorname{Im} \langle\langle d_{1\downarrow} | d^{\dagger}_{1\downarrow} \rangle\rangle_{\omega_2}\right), \tag{62}$$

$$M^{22}_{\downarrow}(\omega) = U^2 \int_{\infty}^{\infty} \mathrm{d}\omega_1\, \mathrm{d}\omega_2 \frac{1 + N(\omega_1) - n(\omega_2)}{\omega - \omega_1 - \omega_2}$$
$$\times \left(-\frac{1}{\pi} \operatorname{Im} \langle\langle S^{\dagger}_1 | S^{-}_1 \rangle\rangle_{\omega_1}\right)\left(-\frac{1}{\pi} \operatorname{Im} \langle\langle d_{1\uparrow} | d^{\dagger}_{1\uparrow} \rangle\rangle_{\omega_2}\right), \tag{63}$$

For M_{33} we obtain the same expressions with the substitution of index 1 by 2,

$$M^{23}_{\uparrow}(\omega) = U^2 \int_{\infty}^{\infty} d\omega_1\, d\omega_2 \frac{1 + N(\omega_1) - n(\omega_2)}{\omega - \omega_1 - \omega_2} \times \left(-\frac{1}{\pi} \operatorname{Im} \langle\langle S_1^- | S_2^+ \rangle\rangle_{\omega_1}\right)\left(-\frac{1}{\pi} \operatorname{Im} \langle\langle d_{1\downarrow} | d_{2\downarrow}^+ \rangle\rangle_{\omega_2}\right), \tag{64}$$

$$M^{23}_{\downarrow}(\omega) = U^2 \int_{\infty}^{\infty} d\omega_1\, d\omega_2 \frac{1 + N(\omega_1) - n(\omega_2)}{\omega - \omega_1 - \omega_2} \times \left(-\frac{1}{\pi} \operatorname{Im} \langle\langle S_1^+ | S_1^- \rangle\rangle_{\omega_1}\right)\left(-\frac{1}{\pi} \operatorname{Im} \langle\langle d_{1\uparrow} | d_{2\uparrow}^+ \rangle\rangle_{\omega_2}\right). \tag{65}$$

Here $N(\omega_1)$ means Bose distribution function. For $M^{32}_{\uparrow\downarrow}$ we must again change index $1 \to 2$. Eqs. (62), (63) and (64), (65) give the complete self-consistent description of nonlocal correlations and quasiparticle interactions for the TIAM. The diagonal elements of the self-energy matrices M_{22} and M_{33} describe single-site inelastic scattering processes; non-diagonal elements M^{23} and M^{32} describe the intersite inelastic scattering processes. As well as the non-diagonal elements of the GMF–GF $\hat{G}^0$, the latter non-diagonal matrix elements are responsible for the specific features of the dynamical behaviour of the TIAM and, more generally, the CIAM.

6. SIAM. Strong correlation

As for the strong correlation regime, even for the SIAM, and in spite of a great number of theoretical efforts, a compact and closed form of the one-particle propagator has not yet been obtained [18–20,51]. The matrix form of our calculation as in the case of the weak correlation will help us to better understand the essence of the difficulties.

In analogy with the Hubbard model [34], for the description of the strong local correlations, we must use a new algebra of operators, namely $\{f_{0\alpha\sigma}\}$ with $\alpha = \pm$,

$$f_{0\alpha\sigma} = n^{\alpha}_{0-\sigma} d_{0\sigma}, \qquad n^{+}_{0\sigma} = n_{0\sigma}, \qquad n^{-}_{0\sigma} = 1 - n_{0\sigma}. \tag{66}$$

In terms of the new operators the relevant matrix GF for the SIAM (23) can be rewritten identically in the following form:

$$\hat{G}_{\sigma}(\omega) = \begin{bmatrix} \langle\langle c_{k\sigma} | c_{k\sigma}^+ \rangle\rangle_{\omega} & \sum_{\beta} \langle\langle c_{k\sigma} | f_{0\beta\sigma}^+ \rangle\rangle_{\omega} \\ \sum_{\alpha} \langle\langle f_{0\alpha\sigma} | c_{k\sigma}^+ \rangle\rangle_{\omega} & \sum_{\alpha\beta} \langle\langle f_{0\alpha\sigma} | f_{0\beta\sigma}^+ \rangle\rangle_{\omega} \end{bmatrix}. \tag{67}$$

To calculate this GF we need to write down the equation of motion for the auxiliary GF, $\hat{\tilde{G}}$,

$$\hat{\tilde{G}}_\sigma(\omega) = \begin{bmatrix} \langle\langle c_{k\sigma} | c^\dagger_{k\sigma} \rangle\rangle_\omega & \langle\langle c_{k\sigma} | f^\dagger_{0+\sigma} \rangle\rangle_\omega & \langle\langle c_{k\sigma} | f^\dagger_{0-\sigma} \rangle\rangle_\omega \\ \langle\langle f_{0+\sigma} | c^\dagger_{k\sigma} \rangle\rangle_\omega & \langle\langle f_{0+\sigma} | f^\dagger_{0+\sigma} \rangle\rangle_\omega & \langle\langle f_{0+\sigma} | f^\dagger_{0-\sigma} \rangle\rangle_\omega \\ \langle\langle f_{0-\sigma} | c^\dagger_{k\sigma} \rangle\rangle_\omega & \langle\langle f_{0-\sigma} | f^\dagger_{0+\sigma} \rangle\rangle_\omega & \langle\langle f_{0-\sigma} | f^\dagger_{0-\sigma} \rangle\rangle_\omega \end{bmatrix}. \tag{68}$$

In the matrix notation the equation of motion reads

$$\hat{E}\hat{\tilde{G}}_\sigma(\omega) - \hat{I} = \hat{D}\,, \tag{69}$$

where

$$\hat{E} = \begin{bmatrix} \omega - \varepsilon_k & -V_k & -V_k \\ 0 & \omega - E_0 - U_+ & 0 \\ 0 & 0 & \omega - E_0 - U_- \end{bmatrix}, \qquad U_\alpha = \begin{cases} U, & \alpha = +\,, \\ 0, & \alpha = -\,, \end{cases} \tag{70}$$

$$\hat{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & n^\dagger_{0-\sigma} & 0 \\ 0 & 0 & n_{-\sigma} \end{bmatrix}, \qquad \hat{D} = \begin{bmatrix} 0 & 0 & 0 \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{bmatrix}. \tag{71}$$

Here $\hat{D}$ is a higher-order GF. As an example we give now two matrix elements,

$$\begin{aligned} D_{22} &= \langle\langle (c_{p\sigma} n_{0-\sigma} + d^\dagger_{0-\sigma} c_{p-\sigma} d_{0\sigma} - c^\dagger_{p-\sigma} d_{0-\sigma} d_{0\sigma}) | f^\dagger_{0+\sigma} \rangle\rangle_\omega\,, \\ D_{33} &= \langle\langle (c_{p\sigma}(1 - n_{0-\sigma}) - d^\dagger_{0-\sigma} c_{p-\sigma} d_{0\sigma} + c^\dagger_{p-\sigma} d_{0-\sigma} d_{0\sigma}) | f^\dagger_{0+\sigma} \rangle\rangle_\omega\,. \end{aligned} \tag{72}$$

Let us introduce the matrix of irreducible GF, $\hat{D}^{\mathrm{ir}}$ in accordance with the definition given in ref. [34],

$$\hat{D}^{\mathrm{ir}} = \hat{D} - \sum_\alpha \binom{A^{+\alpha}}{A^{-\alpha}} (\tilde{G}^{\alpha+}_\sigma \tilde{G}^{\alpha-}_\sigma)\,, \tag{73}$$

where the coefficients $A^{\beta\alpha}$ are determined from the condition

$$\langle [\hat{D}^{\mathrm{ir}}_{\alpha\beta}, f^\dagger_{0\beta\sigma}]_+ \rangle \equiv 0\,. \tag{74}$$

Similarly as in the preceding section we obtain the Dyson equation

$$\hat{\tilde{G}} = \hat{\tilde{G}}^0 + \hat{\tilde{G}}^0 \hat{M} \hat{\tilde{G}}\,, \tag{75}$$

where $\hat{\tilde{G}}^0$ is the generalized mean-field GF. The explicit form of the mean-field renormalizations is as follows:

$$A^{++} = \frac{\langle (d^{\dagger}_{0-\sigma} c_{p-\sigma} + c^{\dagger}_{p-\sigma} d_{0-\sigma})(n_{0\sigma} - n_{0-\sigma}) \rangle}{\langle n_{0-\sigma} \rangle}, \tag{76}$$

$$A^{--} = \frac{-\langle (d^{\dagger}_{0-\sigma} c_{p-\sigma} + c^{\dagger}_{p-\sigma} d_{0-\sigma})(1 + n_{0\sigma} - n_{0-\sigma}) \rangle}{\langle n_{0-\sigma} \rangle}, \tag{77}$$

$$A^{-+} = -A^{++}, \qquad A^{+-} = -A^{--}.$$

The generalized mean-field GF of the d-electrons has the form

$$\ll d_{0\sigma} | d^{\dagger}_{0\sigma} \gg^0_{\omega} = \frac{\langle n_{0-\sigma} \rangle}{\omega - E_0 - U_+ - \Sigma_p V_p A^{++}} \left(1 + \frac{\Sigma_p V_p A^{-+}}{\omega - E_0 - U_-} \right) + \frac{1 - \langle n_{0-\sigma} \rangle}{\omega - E_0 - U_- - \Sigma_p V_p A^{--}} \left(1 + \frac{\Sigma_p V_p A^{+-}}{\omega - E_0 - U_+} \right). \tag{78}$$

For $V_p = 0$, we obtain the exact atomic solution with poles at $E_0 + U_+$ and $E_0 + U_-$,

$$F^{\mathrm{at}}(\omega) = \frac{\langle n_{0-\sigma} \rangle}{\omega - E_0 - U_+} + \frac{1 - \langle n_{0-\sigma} \rangle}{\omega - E_0 - U_-}. \tag{79}$$

The equation corresponding to eq. (78) for the conduction electron GF reads

$$\ll c_{k\sigma} | c^{\dagger}_{k\sigma} \gg^0_{\omega} = \frac{1}{\omega - \varepsilon_k} + \frac{V_k}{\omega - \varepsilon_k} G^0_{21} + \frac{V_k}{\omega - \varepsilon_k} G^0_{31}. \tag{80}$$

Taking into account that

$$(\omega - E_0 - U_+) \ll f_{0+\sigma} | c^{\dagger}_{k\sigma} \gg^0 = \sum_p V_p (\langle n_{0-\sigma} \rangle \ll c_{p\sigma} | c^{\dagger}_{k\sigma} \gg^0), \tag{81}$$

$$(\omega - E_0 - U_-) \ll f_{0+\sigma} | c^{\dagger}_{k\sigma} \gg^0 = \sum_p V_p [(1 - \langle n_{0-\sigma} \rangle) \ll c_{p\sigma} | c^{\dagger}_{k\sigma} \gg^0], \tag{82}$$

we find the following expression for the diagonal element of the conduction electron GF:

$$\ll c_{k\sigma} | c^{\dagger}_{k\sigma} \gg^0_{\omega} = (\omega - \varepsilon_k - |V_k|^2 F^{\mathrm{at}}(\omega))^{-1}. \tag{83}$$

This form of solution also gives the correct expression for $V_k = 0$. The GMF–

GF's (78) and (83) are the essentially new solutions of SIAM in the strongly correlated limit. The paper of ref. [54] is close to our approach; however, the explicit form of the single-particle GF has not been written explicitly. Oh and Doniach [55] calculated the dynamical properties of the SIAM in the context of core-level photoemission spectra. For the mean-field GF they obtained the following result [55]:

$$G^{\sigma}_{\mathrm{dd}}(\omega) = \frac{1 - n_{-\sigma}}{\omega - E_0 - \Sigma_0(\omega)} + \frac{n_{-\sigma}}{\omega - E_0 - U - \Sigma_0(\omega)}, \tag{84}$$

where

$$\Sigma_0(\omega) = \sum_k \frac{|V_k|^2}{\omega - \varepsilon_k}. \tag{85}$$

This solution simply describes the two localized levels E_0 and $E_0 + U$ broadened and shifted due to the mixing potential V_k. Our theory can be considered as a direct generalization of Oh and Doniach's result [55] in the framework of the IGF approach. Of course our eq. (78) is more general than eq. (84) (obtained within the first order in V_k). Also it is important to note that in the atomic limit, when $U \to \infty$ and $V_k \to 0$, the correct functional form of the solution must be recovered. Oh and Doniach [55] found that, for $V_k \geqslant 0.5$ eV, Im $G_{\mathrm{dd}}(\omega)$ starts to go negative for a certain range of ω values, indicating that their decoupling procedure does not conserve probability at each value of ω. Our expression (78) contains complicated correlation functions, which, in principle, must be calculated self-consistently; doing so, the difficulties with the negative spectral density does not appear. For a rough estimation of the behaviour of the correlation functions (eqs. (76), (77)) at low temperatures we can use Oh and Doniach's expression (30) [55], for example ($\mathcal{P}$ meaning the principal part)

$$\begin{aligned}
\langle c^{\dagger}_{k\sigma} d_{0\sigma} \rangle = -\langle c_{k\sigma} d^{\dagger}_{0\sigma} \rangle = (1 - \langle n_{0-\sigma} \rangle) \Bigg(& \theta(-\varepsilon_k) V_k \frac{(\varepsilon_k - E_0 - \Lambda)}{(\varepsilon_k - E_0 - \Lambda)^2 + \Delta^2} \\
& + \frac{V_k}{\pi} \int_{-B}^{M} \mathcal{P} \frac{\mathrm{d}\omega}{(\omega - \varepsilon_k)} \frac{\Delta}{(\omega - E_0 - \Lambda)^2 + \Delta^2} \Bigg) \\
& + \langle n_{0-\sigma} \rangle \Bigg(\theta(-\varepsilon_k) V_k \frac{(\varepsilon_k - E_0 - U - \Delta)}{(\varepsilon_k - E_0 - U - \Lambda)^2 + \Delta^2} \\
& + \frac{V_k}{\pi} \int_{-B}^{M} \mathcal{P} \frac{\mathrm{d}\omega}{(\omega - \varepsilon_k)} \frac{\Delta}{(\omega - E_0 - U - \Lambda)^2 + \Delta^2} \Bigg)
\end{aligned} \tag{86}$$

and

$$\langle c_K^\dagger n_{0-\sigma} d_{0\sigma} \rangle = -\langle c_{k\sigma} n_{0-\sigma} d_{0\sigma}^\dagger \rangle$$
$$= \langle n_{0-\sigma} \rangle V_k \Big(\theta(-\varepsilon_k) \frac{(\varepsilon_k - E_0 - U - \Lambda)}{(\varepsilon_k - E_0 - U - \Lambda)^2 + \Delta^2}$$
$$+ \frac{1}{\pi} \int_{-B}^{M} \mathscr{P} \frac{\mathrm{d}\omega}{(\omega - \varepsilon_k)} \frac{\Delta}{(\omega - E_0 - U - \Lambda)^2 + \Delta^2} \Big) , \tag{87}$$

where

$$\Sigma_0(\omega) = \Lambda(\omega) + \mathrm{i}\Delta(\omega) . \tag{88}$$

The set of eqs. (76)–(78) and (86)–(87) completely solve the GMF description of SIAM in the strongly correlated case. It is worthy to note that after substitution of (86) and (87) into (76) and (77) we obtain the GF (78) at the second order in V_k. In addition, our theory allows to calculate inelastic scattering corrections which are described by the self-energy operator

$$\hat{M} = \hat{I}^{-1} \left\{ \sum_{pq} V_p V_q \begin{bmatrix} 0 & 0 & 0 \\ 0 & M_{22} & M_{23} \\ 0 & M_{32} & M_{33} \end{bmatrix} \right\} \hat{I}^{-1} , \tag{89}$$

where

$$M_{22} = {}^{\mathrm{ir}}\langle\langle Y_{22} | Y_{22}^\dagger \rangle\rangle^{\mathrm{ir}} , \qquad M_{33} = {}^{\mathrm{ir}}\langle\langle Y_{33} | Y_{33}^\dagger \rangle\rangle^{\mathrm{ir}} ,$$
$$Y_{22} = c_{p\sigma} n_{0-\sigma} + d_{0-\sigma}^\dagger c_{p-\sigma} d_{0\sigma} - c_{p-\sigma}^\dagger d_{0-\sigma} d_{0\sigma} , \tag{90}$$
$$Y_{33} = c_{p\sigma}(1 - n_{0-\sigma}) - d_{0\sigma}^\dagger c_{p-\sigma} d_{0\sigma} + c_{p-\sigma}^\dagger d_{0-\sigma} d_{0\sigma} .$$

The complete solution of the Dyson equation in the form of (75) is very complicated. Nevertheless it is possible to write down the simplest approximate solution which includes the inelastic scattering corrections

$$\langle\langle d_{0\sigma} | d_{0\sigma}^\dagger \rangle\rangle_\omega \approx \frac{\langle n_{0-\sigma} \rangle}{\omega - E_0 - U - \Sigma_p V_p A^{++} - \tilde{M}_{22}(\omega)} \Big(1 + \frac{\Sigma_p V_p A^{-+}}{\omega - E_0 - \tilde{M}_{22}(\omega)} \Big)$$
$$+ \frac{1 - \langle n_{0-\sigma} \rangle}{\omega - E_0 - \Sigma_p V_p A^{--} - \tilde{M}_{33}(\omega)}$$
$$\times \Big(1 + \frac{\Sigma_p V_p A^{+-}}{\omega - E_0 - U - \tilde{M}_{33}(\omega)} \Big) . \tag{91}$$

The calculation of higher-order GF's which describe the inelastic scattering corrections (90) can be done in the same way as in the previous sections 4 and 5.

7. TIAM. Strong correlation

In the preceding sections we have considered a self-consistent description of the dynamical behaviours of (i) the TIAM in the case of weak correlations, and (ii) the SIAM in the case of strong correlations. In this section we will examine the case of the very strong Coulomb correlations for the TIAM. For this aim it is convenient to use the relevant algebra of Hubbard's operators X_i^{mn} [56,57]. The TIAM Hamiltonian takes then the following form ($U \to \infty$):

$$H = \sum_{km} \varepsilon_{km} c_{km}^{\dagger} c_{km} + \sum_{im} E_{0m} X_i^{mm} + \sum_i E_{f0} X_i^{00} + \frac{1}{\sqrt{N}} \sum_{jkm} (V_{km}^{*} \, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_j} c_{km}^{\dagger} X_j^{0m} + \mathrm{h.c.}) , \qquad i = 1,2 . \tag{92}$$

As it has been mentioned above, a more symmetric form of the problem can be handled by using a new set of variables,

$$X_{\pm}^{0m} = \frac{1}{\sqrt{2}} (X_1^{0m} \pm X_2^{0m}) , \qquad X_1^{0m} = \frac{1}{\sqrt{2}} (X_+^{m0} + X_-^{m0}) ,$$
$$X_2^{0m} = \frac{1}{\sqrt{2}} (X_+^{m0} - X_-^{m0}) . \tag{93}$$

In terms of the so-called "odd" and "even" variables the full Hamiltonian of the TIAM can be rewritten as

$$H = H_0 + H_1 , \tag{94}$$

where

$$H_0 = \sum_{km} \varepsilon_{km} c_{km}^{\dagger} c_{km} + \sum_m E_{0m} (X_1^{mm} + X_2^{mm}) + E_{f0} (X_1^{00} + X_2^{00}) , \tag{95}$$

$$H_1 = \frac{1}{\sqrt{N}} \sum_{km} (V_{k+} c_{km}^{\dagger} X_+^{0m} + V_{k-} c_{km}^{\dagger} X_-^{0m} + \mathrm{h.c.}) . \tag{96}$$

The new hybridization matrix element is expressed as

$$V_{k\pm} = \frac{1}{\sqrt{2}} V(1 \pm \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}) , \tag{97}$$

the two impurities being located on the z axis at $-R/2$ and $+R/2$. The convenience of the even and odd operators representation is obvious. The relevant matrix GF is a 3×3 matrix (instead of a 5×5 matrix by using the same algebra of operators as in section 6),

$$\hat{G} = \begin{bmatrix} \langle\langle c_{km}|c^{\dagger}_{km}\rangle\rangle & \langle\langle c_{km}|X^{m0}_{+}\rangle\rangle & \langle\langle c_{km}|X^{m0}_{-}\rangle\rangle \\ \langle\langle X^{0m}_{+}|c^{\dagger}_{km}\rangle\rangle & \langle\langle X^{0m}_{+}|X^{m0}_{+}\rangle\rangle & \langle\langle X^{0m}_{+}|X^{m0}_{-}\rangle\rangle \\ \langle\langle X^{0m}_{-}|c^{\dagger}_{km}\rangle\rangle & \langle\langle X^{0m}_{-}|X^{m0}_{+}\rangle\rangle & \langle\langle X^{0m}_{-}|X^{m0}_{-}\rangle\rangle \end{bmatrix} . \tag{98}$$

From the comparison of eqs. (68) and (98) we can see that the new set of variables (even and odd) somewhat allows to consider the TIAM in terms of the SIAM. However, this "reduction" from TIAM to SIAM is only partial, as we will see later. The equation of motion for the GF (98) can then be written in the form

$$\hat{E}\hat{G}_{\sigma}(\omega) - \hat{I} = \hat{D} , \tag{99}$$

where

$$\hat{E} = \begin{bmatrix} \omega - \varepsilon_k & 0 & 0 \\ 0 & \omega - E_{0m} & 0 \\ 0 & & \omega - E_{0m} \end{bmatrix} , \qquad \hat{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \Delta^{+}_{mm} & 0 \\ 0 & 0 & \Delta^{-}_{mm} \end{bmatrix} , \tag{100}$$

$$\Delta^{\pm}_{mm} = \langle X^{00}_{\pm}\rangle + \langle X^{mm}_{\pm}\rangle , \tag{101}$$

$$\hat{D} = \begin{bmatrix} 0 & 0 & 0 \\ \phi_{21} & \phi_{22} & \phi_{23} \\ \phi_{21} & \phi_{32} & \phi_{33} \end{bmatrix} , \tag{102}$$

$$\phi_{21} = \frac{1}{\sqrt{N}} \sum_{pn} V^{*}_{p+} \langle\langle \Delta^{+}_{mn} c_{pn} | c^{\dagger}_{km}\rangle\rangle , \qquad \phi_{22} = \frac{1}{\sqrt{N}} \sum_{pn} V^{*}_{p+} \langle\langle \Delta^{+}_{mn} c_{pn} | X^{m0}_{+}\rangle\rangle ,$$

$$\phi_{23} = \frac{1}{\sqrt{N}} \sum_{pn} V^{*}_{p+} \langle\langle \Delta^{+}_{mn} c_{pn} | X^{m0}_{-}\rangle\rangle , \qquad \phi_{31} = \frac{1}{\sqrt{N}} \sum_{pn} V^{*}_{p-} \langle\langle \Delta^{-}_{mn} c_{pn} | c^{\dagger}_{km}\rangle\rangle ,$$

$$\phi_{32} = \frac{1}{\sqrt{N}} \sum_{pn} V^{*}_{p-} \langle\langle \Delta^{-}_{mn} c_{pn} | X^{m0}_{+}\rangle\rangle , \qquad \phi_{33} = \frac{1}{\sqrt{N}} \sum_{pn} V^{*}_{p-} \langle\langle \Delta^{-}_{mn} c_{pn} | X^{m0}_{-}\rangle\rangle . \tag{103}$$

The method to introduce the irreducible parts for the TIAM in the case of strong correlations is the same as for eq. (73). We follow here the same approach. The coefficients $A^{\alpha\beta}$ are determined from the condition

$$\langle [D^{\mathrm{ir}}_{\alpha\beta}, X^{m0}_{\beta}]_+ \rangle \equiv 0 \,. \tag{104}$$

For example, let us calculate the coefficient A^{++}_{22} (compare with eq. (76)),

$$\langle [\Phi^{\mathrm{ir}}_{22}, X^{m0}_{+}]_+ \rangle = \langle [(\Delta^{+}_{mn} c_{pn})^{\mathrm{ir}}, X^{m0}_{+}]_+ \rangle = A^{++}_{22} \langle [X^{0m}_{+}, X^{m0}_{+}]_+ \rangle \,,$$
$$A^{++}_{22} = \frac{\langle [\Delta^{\dagger}_{mn} c_{pn}, X^{m0}_{+}]_+ \rangle}{\langle [X^{0m}_{+}, X^{m0}_{+}]_+ \rangle} = \frac{\langle \delta_{mn} (X^{m0}_{+} - X^{0m}_{+}) c_{pn} \rangle}{\langle \Delta^{+}_{mm} \rangle} \,. \tag{105}$$

The GMF Green's function is defined as

$$\hat{E}\hat{G}^{0} = \hat{I} \,. \tag{106}$$

From this equation one can find that

$$\langle\langle X^{0m}_{+} | X^{m0}_{+} \rangle\rangle^{0}_{\omega} = \frac{\langle \Delta^{+}_{mm} \rangle}{\left[\omega - E_{0m} - \frac{1}{\sqrt{N}} \sum_{pn} V^{*}_{p+} \left(\frac{\langle \delta_{mn} (X^{m0}_{+} - X^{0m}_{+}) c_{pn} \rangle}{\langle \Delta^{+}_{mm} \rangle} \right) \right]} \,, \tag{107}$$

$$\langle\langle X^{0m}_{-} | X^{m0}_{-} \rangle\rangle^{0}_{\omega} = \frac{\langle \Delta^{-}_{mm} \rangle}{\left[\omega - E_{0m} - \frac{1}{\sqrt{N}} \sum_{pn} V^{*}_{p-} \left(\frac{\langle \delta_{mn} (X^{m0}_{-} - X^{0m}_{-}) c_{pn} \rangle}{\langle \Delta^{+}_{mm} \rangle} \right) \right]} \,, \tag{108}$$

and the equation for conduction electron GF,

$$\langle\langle c_{km} | c^{\dagger}_{km} \rangle\rangle^{0}_{\omega} = \frac{1}{\omega - \varepsilon_k} + \frac{V_{k+}}{\omega - \varepsilon_k} \frac{1}{\sqrt{N}} \sum_{pn} V^{*}_{p+} \frac{\langle \Delta^{+}_{mm} \rangle}{\omega - E_{0m}} \langle\langle c_{pn} | c^{\dagger}_{km} \rangle\rangle^{0}_{\omega}$$
$$+ \frac{V_{k-}}{\omega - \varepsilon_k} \frac{1}{\sqrt{N}} \sum_{pn} V^{*}_{p-} \frac{\langle \Delta^{-}_{mm} \rangle}{\omega - E_{0m}} \langle\langle c_{pn} | c^{\dagger}_{km} \rangle\rangle^{0}_{\omega} \,. \tag{109}$$

If we take in the r.h.s. of eq. (109) the diagonal elements, i.e. terms proportional to $\delta pk\, \delta mn$ we easily find

$$\langle\langle c_{km} | c^{\dagger}_{km} \rangle\rangle^{0}_{\omega} \approx \frac{1}{\omega - \varepsilon_k - (|V_{k+}|^2 \langle \Delta^{+}_{mm} \rangle + |V_{k-}|^2 \langle \Delta^{-}_{mm} \rangle)/(\omega - E_{0m})} \,. \tag{110}$$

In the case of $V_{k\pm} = 0$, this expression corresponds to an exact solution

$$\langle\langle c_{km} | c_{km}^{\dagger} \rangle\rangle = \frac{1}{\omega - \varepsilon_k} . \tag{111}$$

Using the definition of $\hat{G}^0$ as previously considered it is then possible to derive the approximate Dyson equation

$$\hat{G} = \hat{G}^0 + \hat{G}^0 \hat{M} \hat{G} . \tag{112}$$

The self-energy operator is given by the second order in $V_{k\pm}$,

$$M \approx \frac{1}{N} \sum_{pn} \sum_{ql} \hat{W}_p \overset{\approx}{M}{}_{pq}^{nl} W_q . \tag{113}$$

The matrix $\overset{\approx}{M}{}_{pq}^{nl}$ has a similar form as eq. (89) and all further considerations (section 6) can be again performed here as for the SIAM. The difference now consists of the non-diagonal terms of self-energy operators M_{23} and M_{32}. In analogy with eqs. (64) and (65) they contain higher-order GF's which describe inelastic impurity–impurity correlations terms. In order to obtain an approximate estimation of higher-order correlators contained in eq. (113), it is possible to use any relevant expression since the functional structure of dynamical TIAM solutions has the right general form. A more consistent approach would need to calculate the collective correlation function independently, like transversal spin susceptibility $\langle\langle S_1^{\pm} | S_2^{\mp} \rangle\rangle_{\omega}$. We plan to look into this aspect of the problem in the future.

8. Concluding remarks

In summary, we have developed a new approach to describe the many-body dynamics of SIAM and TIAM in the framework of the IGF formalism. We have obtained a new interpolation solution, the one-particle GF's for the SIAM and TIAM as well as the solution for the PAM in the weakly correlated case. In this last case the functional of the generalized mean-fields only depends on the mean densities of electrons. Moreover our solution improves the H–F solution; it allows to incorporate (i) the correlation of the spin-up and spin-down electrons at the impurity level as well as (ii) the impurity–impurity correlation effects in the case of the TIAM. As far as strong Coulomb correlations are concerned we have obtained essentially new solutions. Furthermore we are then able to confirm the statement [34–36,38–40] that in this case the mean-field renormalizations have a quite nontrivial structure and

cannot be reduced to the mean density functional. The theory we suggest allows to find explicitly the damping of quasiparticle excitations in a self-consistent way as was demonstrated here.

In order to give a complete picture of the role of non-local or impurity–impurity correlations we must extract the Kondo-type peak of the spectral density of states in the strongly correlated case for low temperatures. For the SIAM there are a few reasonable schemes on how to do so [51,58,59]. For the TIAM this type of behaviour has not yet been described analytically. There are only a few numerical calculations [60,61] within quantum Monte-Carlo algorithm which gives some useful insights into the considered problem. However it is evident that for the TIAM (or for the CIAM [66]) the definition of the Kondo effect, which is associated with the screening of a single impurity spin at a characteristic temperature T_k, must be redefined. An approach which permits to define the renormalized Kondo temperature in the presence of additional impurities has been proposed many years ago [23] within the framework of a perturbation theory. The main assumption of ref. [23] is that, at the impurity site i, the logarithmic contribution which characterizes a Kondo system undergoes a transformation such that

$$\ln T \to \ln(T^2 + W^2)^{1/2} \tag{114}$$

under the influence W of interacting impurities around i. So, as emphasized by the authors of ref. [23], the single-impurity treatment is almost valid and needs only small corrections in the dilute limit. However, a more correct way to define the Kondo temperature in the $U \to \infty$ limit of the Anderson model is related to the low temperature behaviour of the spin susceptibility [1,62]

$$\chi \sim \frac{1}{2\pi T_k}, \tag{115}$$

where in the symmetrical case the Kondo temperature is

$$T_k = \frac{(2U\Gamma)^{1/2}}{\pi} e^{-\pi U/8\Gamma}. \tag{116}$$

In the region where T_k is of the same order as T_{RKKY} the role of non-local correlations is strongly increased and the correct definition of the Kondo temperature is a very nontrivial problem. The various cluster Anderson models confirm the necessity of adapted definitions of the Kondo temperature. For example in ref. [31], where the Anderson cluster has been considered, the Kondo temperature is defined to be the triplet–singlet splitting, and in this model is given by (see also [8] and [50])

$$T_k = \frac{4V^2}{\varepsilon_1 - \varepsilon_f}. \tag{117}$$

The nonexponential dependence of the Kondo temperature on the hybridization follows from modeling the continuous spectrum of band energies by only a few discrete states. In the region of interplay between RKKY and Kondo behaviours the key point is then to connect the partial Kondo screening effect with the low temperature behaviour of the total spin susceptibility. The non-local contributions to the total spin susceptibility of two very well formed impurity magnetic moments have been calculated by ref. [63] (see also [6,64]),

$$\chi_{\text{pair}} \sim 2\chi - 12\,\pi E_F \left(\frac{\chi}{g\mu_B}\right)^2 \frac{\cos(2k_F R)}{(k_F R)^3}. \tag{118}$$

The problem is how to find an interpolated expression of the susceptibility in the region of RKKY–Kondo interplay. As it is well known, it is extremely difficult to describe such a threshold behaviour analytically. However, progress is expected both from analytical and numerical investigation in this fascinating field.

Acknowledgements

One of the authors (A.L.K) gratefully acknowledges Swiss National Science Foundation and French Ministère de la Recherche et de la Technologie for the partial financial support during this work.

References

[1] A.M. Tsvelik and P.B. Wiegmann, Adv. Phys. 32 (1983) 453.
[2] N. Andrei, K. Furuya and J.H. Lowenstein, Rev. Mod. Phys. 55 (1983) 331.
[3] A.J. Heeger, Phys. Rev. Lett. 22 (1969) 1420.
[4] B.R. Coles, Physica B 91 (1977) 167.
[5] B.R. Coles, B.V. Sarkissian and R.H. Taylor, Philos. Mag. B 37 (1978) 489.
[6] J.C. Parlebas and F. Gautier, J. Phys. F 4 (1974) 1044.
[7] J.C. Parlebas, J. Low Temp. Phys. 19 (1975) 317.
[8] P. Fulde, J. Keller and G. Zwicknagl, Solid State Phys. 41 (1988) 1.
[9] S. Doniach, Physica B 91 (1977) 231.
[10] S. Doniach, Phys. Rev. B 35 (1987) 1814.
[11] J.W. Allen, M.B. Maple, J.S. Kang, K.N. Yang, M.S. Torikachvili, Y. Lassaily, W.P. Ellis, B.B. Pate and I. Linday, Phys. Rev. 41 (1990) 9013.
[12] S. Rahman, T. Mihalisin, J.E. Crow and P. Schlottmann, Solid State Commun. 75 (1990) 279.

[13] J.P. Mignot, Ph. Boutrouille, L.P. Regnault, P. Maen and P. Lejay, Solid State Commun. 77 (1991) 317.
[14] F. Steglich, G. Sparn, R. Moog, S. Horn, A. Grauel, M. Lang, M. Nowak, A. Loidl, A. Krimmel, K. Knorr, A.P. Murani and M. Tachiki, Physica B 163 (1990) 19.
[15] W.P. Beyermann, M.F. Hundley, P.C. Canfield, J.D. Thompson, Z. Fisk, J.L. Smith, M. Selsane, C. Godart and M. Latroche, Phys. Rev. Lett. 66 (1991) 11057.
[16] J.M. Lawrence, M.F. Hundley, J.D. Thompson, G.G. Kwei and Z. Fisk, Phys. Rev. B 43 (1991) 11057.
[17] I. Das and E.V. Sampathkumaran, Solid State Commun. 81 (1992) 905.
[18] G. Czycholl, Phys. Rep. 143 (1986) 277.
[19] D.M. Newns and N. Read, Adv. Phys. 36 (1987) 799.
[20] Th. Pruschke and N. Grewe, Z. Phys. B 74 (1989) 439.
[21] C.I. Kim, Y. Kuramoto and T. Kasuya, J. Phys. Soc. Jpn. 59 (1990) 2414.
[22] M. Marinaro, C. Noce and A. Romano, J. Phys. Condens. Matt. 3 (1991) 3719.
[23] Y.C. Tsay and M.W. Klein, Phys. Rev. B 11 (1975) 318.
[24] K. Schönhammer and O. Gunnarsson, J. Magn. Magn. Mat. 63–64 (1987) 481.
[25] E. Abrahams, J. Magn. Magn. Mat. 63–64 (1987) 234.
[26] B.A. Jones, B.G. Kotliar and A.J. Millis, Phys. Rev. B 39 (1989) 3415.
[27] B.A. Jones and C. Varma, Phys. Rev. B 40 (1989) 324.
[28] T. Yanagisawa, J. Phys. Soc. Jpn. 60 (1991) 29.
[29] O. Sakai, Y. Shimizu and T. Kasuya, Solid State Commun. 75 (1990) 81.
[30] L.C. Andreani, S. Fraizzoli and H. Beck, Solid State Commun. 77 (1991) 635.
[31] L.C. Andreani and H. Beck, Solid State Commun. 79 (1991) 17.
[32] T. Saso, Phys. Rev. B 44 (1991) 450.
[33] C.N. Yang, Phys. Rev. Lett. 19 (1967) 1312.
[34] A.L. Kuzemsky, Teor. Mat. Fiz. 36 (1978) 208; Sov. Phys. Theor. Math. Phys. 36 (1978) 692.
[35] A.L. Kuzemsky, Doklady Akad. Nauk SSSR 309 (1989) 323.
[36] A.L. Kuzemsky, Phys. Lett. A 153 (1991).
[37] P.W. Anderson, Phys. Rev. 124 (1961) 41.
[38] D. Marvakov, A.L. Kuzemsky and J. Vlahov, J. Phys. C 18 (1985) 2871.
[39] D. Marvakov, A.L. Kuzemsky and J. Vlahov, Physica B 138 (1986) 129.
[40] A.L. Kuzemsky, in: Proc. V Int. Symp. on Selected Topics in Statistical Mechanics (World Scientific, Singapore, 1990) p. 157.
[41] J. Friedel, Nuovo Cimento 52 (1958) 287; J. Phys. Radium 23 (1962) 501.
[42] A. Blandin, J. Appl. Phys. 39 (1968) 1285.
[43] S. Alexander and P.W. Anderson, Phys. Rev. A 133 (1964) 1594.
[44] J.R. Schrieffer and D.C. Mattis, Phys. Rev. A 140 (1965) 1412.
[45] B. Kjöllerström, D.J. Scalapino and J.R. Schrieffer, Phys. Rev. 148 (1966) 665.
[46] B.A. Jones and C.M. Varma, Phys. Rev. Lett. 58 (1987) 843.
[47] B.A. Jones, C.M. Varma and J.W. Wilkins, Phys. Rev. Lett. 61 (1988) 125.
[48] M. Takeshige, O. Sakai, T. Kasuya, J. Phys. Soc. Jpn. 60 (1991) 666;
A. Kotani, T. Jo and J.C. Parlebas, Adv. Phys. 37 (1988) 37.
[49] M.W. Long, J. Phys. Condens. Matt. 1 (1989) 10321.
[50] J.C. Parlebas, Phys. Stat. Sol. b 160 (1990) 11.
[51] P. Coleman, Phys. Rev. B 35 (1987) 5072.
[52] D.N. Zubarev, Uspeckhi Fiz. Nauk 71 (1960) 71.
[53] B. Caroli, J. Phys. Chem. Sol. 28 (1967) 1427.
[54] L.M. Roth, J. Appl. Phys. 40 (1969) 1103.
[55] S.J. Oh and S. Doniach, Phys. Rev. B 26 (1982) 2085.
[56] J. Hubbard, Proc. R. Soc. A 285 (1965) 542.
[57] N. Grewe and H. Keiter, Phys. Rev. B 28 (1981) 4420.
[58] C. Lacroix, J. Phys. F 11 (1981) 2389.
[59] G. Czycholl, Phys. Rev. B 31 (1985) 2867.

[60] R.M. Fye and J.E. Hirsch, Phys. Rev. B 40 (1990) 4780.
[61] R.M. Fye, Phys. Rev. B 41 (1990) 2490.
[62] C. Jayaprakash, H.R. Krishna-Murthy and J.W. Wilkins, J. Appl. Phys. 53 (1982) 2142.
[63] M. Ishii, Prog. Theor. Phys. 55 (1976) 1373.
[64] K. Yamada, Prog. Theor. Phys. 62 (1979) 901.
[65] L.M. Falicov, in: Recent Progress in Many-Body Theories, vol. 1 (Plenum Press, New York 1988).
[66] J. Callaway, D.P. Chen and Y. Zhang, Phys. Rev. B 36 (1987) 2084.