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NEW INTERPOLATIVE TREATMENT OF THE SINGLE-IMPURITY ANDERSON MODEL

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The many-body problem and, in particular, the study of correlated, strongly interacting electrons in solids is one of the most fascinating subjects in solid state physics. [1, 2]. 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-Tc superconductors). The behaviour of electrons in these materials exhibit both localized and delocalized features [3], [4]. Contrary to the wide-band electron systems (like simple metals), where the fundamentals are very well known and the electrons can be represented as only weakly interacting, in these substances the bands are narrow and the electrons interact strongly giving rise to complicated spectra and interesting and important phenomena like band magnetism, strong effective mass renormalizations and superconductivity.

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) [5] and Hubbard model [6]. In spite of certain unrealistic simplifications these models exhibit the key physical feature: the competition and interplay between kinetic energy (itinerant) and potential energy (localized) effects (c.f. [7]). A fully consistent theory of the quasiparticle dynamics of both models is believed to be crucially important [8] 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 a satisfactory solution of the dynamical problem is still missing for the "simple" Anderson/Hubbard model. The famous Bethe-ansatz solutions of the Hubbard model in one dimension determination of the ground state and thermodynamic (static) properties (static susceptibility, specific heat etc.). But for both models there is not yet an exact solution for the many-body dynamics. Therefore, it is still necessary and justified to develop improved approximations for the dynamical properties of the SIAM.

The present paper is devoted to the development of such an improved interpolating approximation for the dynamical properties of the SIAM. We will show that a self-consistent many-body approximation can be formulated which reproduces all relevant exactly solvable limits of the model and interpolates between the strong-coupling and the weak-coupling limit.

The Hamiltonian of the SIAM can be written in the form

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

where $c^{\dagger}_{\vec{k}\sigma}$ and $f^{\dagger}_{0\sigma}$ are the creation operators for conduction and localized electrons; $\epsilon_{\vec{k}}$ is the conduction electron energy dispersion, $E_{0\sigma}$ is the localized (f-) electron energy level and U is the intra-atomic Coulomb interaction at the impurity site. V represents the $s-f$ hybridisation.

In connection with the dynamical properties the one-particle Green function is the basic quantity to be calculated. The two-time thermodynamic Green Function (GF) of the localized electrons is defined by

$$G_\sigma(t) = << f_{0\sigma}(t) | f^\dagger_{0\sigma} >> = -i\theta(t) < [f_{0\sigma}(t), f^\dagger_{0\sigma}]_+ > \qquad (2)$$

We start by considering the equations of motion for the Fourier transformed, frequency-dependent GF:

$$\begin{aligned}(z - E_{0\sigma} - \Delta(z)) << f_{0\sigma} | f^\dagger_{0\sigma} >>_z &= 1 + U << f_{0\sigma} f^\dagger_{0-\sigma} f_{0-\sigma} | f^\dagger_{0\sigma} >>_z \\ &= 1 + \Sigma_\sigma(z) << f_{0\sigma} | f^\dagger_{0\sigma} >>_z \qquad (3)\end{aligned}$$

where the latter equation defines the one-particle selfenergy $\Sigma_\sigma(z)$ and

$$\Delta(z) = \sum_k \frac{|V|^2}{z - \epsilon_{\vec{k}}}$$

has been used.

The higher order Green function in Eq.3 fulfills the equation of motion

$$\begin{aligned}(z - E_{0\sigma} - U) << f_{0\sigma} f^\dagger_{0-\sigma} f_{0-\sigma} | f^\dagger_{0\sigma} >>_z &= < f^\dagger_{0-\sigma} f_{0-\sigma} > \\ + V \sum_k (<< c_{\vec{k}\sigma} f^\dagger_{0-\sigma} f_{0-\sigma} | f^\dagger_{0\sigma} >>_z &- << c_{\vec{k}-\sigma} f^\dagger_{0-\sigma} f_{0\sigma} | f^\dagger_{0\sigma} >>_z \\ &+ << c^\dagger_{\vec{k}-\sigma} f_{0\sigma} f_{0-\sigma} | f^\dagger_{0\sigma} >>_z) \qquad (4)\end{aligned}$$

¿From these two exact equations one immediately recovers the two trivial, exactly solvable limits of the SIAM, namely

$$\begin{aligned}G_\sigma(z) &= \frac{1 - < f^\dagger_{0-\sigma} f_{0-\sigma} >}{z - E_{0\sigma}} + \frac{< f^\dagger_{0-\sigma} f_{0-\sigma} >}{z - E_{0\sigma} - U}, \text{ for V} = 0 \\ G_\sigma(z) &= G_0(z) = \frac{1}{z - E_{0\sigma} - \Delta(z)}, \text{ for U} = 0 \qquad (5)\end{aligned}$$

We want to develop an "interpolating" solution for the SIAM, i.e. a solution which recovers these two limits, which – in analogy with the terminology known from the Hubbard model– we call "atomic limit" ($V = 0$) and "band limit" ($U = 0$). The simplest approximative "interpolating" solution has the form [12, 13]:

$$\begin{aligned}G_\sigma(z) &= \frac{1}{z - E_{0\sigma} - \Delta(z)} + \frac{U < f^\dagger_{0-\sigma} f_{0-\sigma} >}{(z - E_{0\sigma} - \Delta(z) - U)(z - E_{0\sigma} - \Delta(z))} \\ &= \frac{1 - < f^\dagger_{0-\sigma} f_{0-\sigma} >}{z - E_{0\sigma} - \Delta(z)} + \frac{< f^\dagger_{0-\sigma} f_{0-\sigma} >}{z - E_{0\sigma} - \Delta(z) - U} \qquad (6)\end{aligned}$$

. This is equivalent to a selfenergy fulfilling the equation

$$\Sigma_\sigma(z) = \frac{U < f^\dagger_{0-\sigma} f_{0-\sigma} >}{1 - (U - \Sigma_\sigma(z)) G_\sigma(z)} = \frac{U < f^\dagger_{0-\sigma} f_{0-\sigma} >}{1 - U(1 - < f^\dagger_{0-\sigma} f_{0-\sigma} >) G_0(z)} \qquad (7)$$

Obviously, this is just the analogue of the Hubbard III approximation [14] for the SIAM. As for the Hubbard model, however, Fermi liquid properties and the Friedel sum rule, which should also hold for the SIAM [15] at least order by order within the standard U-perturbation theory, are violated within this simple approximation (6).

An approximation, which automatically fulfills these Fermi liquid properties and sum rules, is provided by the selfconsistent second order U-perturbation treatment (SOPT). Within this weak-coupling expansion up to order U^2 the selfenergy is given by

$$\begin{aligned}\Sigma_\sigma(z) = U < f^\dagger_{0-\sigma} f_{0-\sigma} > + \left(-\frac{1}{\pi}\right)^3 U^2 \int_{-\infty}^{\infty} dE_1 \int_{-\infty}^{\infty} dE_2 \int_{-\infty}^{\infty} dE_3 \\ \frac{f(E_1) f(E_2)(1 - f(E_3)) + (1 - f(E_1))(1 - f(E_2)) f(E_3)}{z - E_1 - E_2 + E_3} \\ \times Im G_\sigma(E_1) Im G_{-\sigma}(E_2) Im G_{-\sigma}(E_3) \qquad (8)\end{aligned}$$

One of the goals of the present paper is to find some way to incorporate this U^2 perturbation theory expansion in the functional structure of the interpolating dynamical solution of the SIAM. This means that the approximation we are looking for shall not only fulfill the limits (5), but the approximation for the selfenergy shall be correct up to order U^2 perturbationally around the band limit $U = 0$. On the other hand also the atomic limit $V = 0$ shall be fulfilled. This is the case for the SOPT around the Hartree-Fock solution [16], but only for the symmetric SIAM. For the general situation (position of the Fermi level relative to E_0 and $E_0 + U$) a heuristic semi-empirical approach for constructing such an approximation has been presented for the Anderson model in Ref.[17] and for the Hubbard model in Refs.[18, 19]; the latter approximation [18] can also easily be applied to the SIAM. Our intention is to take into account expansion (8) self-consistently. Furthermore, in contrast to Refs. [16, 17, 18] the approximation shall not only fulfill the atomic limit $V = 0$, but it shall be correct up to order V^2 in a strong-coupling expansion around the atomic limit.

During the last decades several different refined many-body techniques have been applied to the SIAM [20] - [38], and many of these approaches are strong-coupling treatments around the atomic limit and can be classified as being correct up to a certain power in the hybridization V. This is, in particular, true for the non-crossing approximation (NCA), which is correct at least up to order V^4 and may be considered to be the most successful approximate treatment of the SIAM [21, 22, 23, 24, 25, 26, 27]. The NCA takes into account an infinite order resummation of

all non-crossing diagrams within a systematic perturbation treatment with respect to the hybridisation V in terms of Goldstone diagrams. Originally this method was formulated for the $U \to \infty$ SIAM, but meanwhile also finite U versions of the NCA exist [28, 29]. The NCA fails, however, to correctly reproduce the weak-coupling limit for small U, and Fermi liquid sum rules are violated. This is still true for the even more sophisticated post-NCA developped recently by Anders and Grewe [30]. Similar statements can be made for a higher order equation of motion decoupling scheme [31, 32, 33]; it is correct up to order V^2 around the atomic limit and has so far been applied only in the limit $U \to \infty$, but can easily be extended to the case of finite U. But then it is easy to see that it fails to reproduce the SOPT of Eq. 8, and – also for infinite U – the Fermi liquid sum rules are violated. An alternative advanced many-body approximation was suggested and investigated by Neal [34]; this treatment correctly reproduces both limits (5) and is obviously (from the structure of the expression for the Green function) a direct, systematic improvement of (6) and is correct up to order V^2, but it does not incorporate the SOPT (8), too.

When mentioning the progress achieved for an understanding of the many-body dynamics of the SIAM one should not forget the important numerical results obtained by the numerical renormalization group treatment [39] and by quantum Monte-Carlo methods [40]. Though a real understanding of the SIAM can only be reached within an analytical theory, the available numerical results for the frequency dependence of the spectral function, for instance, are very useful, in particular as they allow for a comparison with the results of an analytical approach.

To construct a suitable approximate solution for the SIAM fulfilling all desired properties mentioned above we start from the following exact relation [36]:

$$<< f_{0\sigma} | f^\dagger_{0\sigma} >>_z = G_0(z) + G_0(z) P(z) G_0(z) \qquad (9)$$

$$P(z) = U < f^\dagger_{0-\sigma} f_{0-\sigma} > + U^2 << f_{0\sigma} f^\dagger_{0-\sigma} f_{0-\sigma} | f^\dagger_{0\sigma} f^\dagger_{0-\sigma} f_{0-\sigma} >>_z \qquad (10)$$

The equation (9) is still exact. To construct a suitable approximation for the higher-order GF (10) we consider the equation of motion for it:

$$\begin{aligned}(z - E_{0\sigma} - U) << f_{0\sigma} f^\dagger_{0-\sigma} f_{0-\sigma} | f^\dagger_{0\sigma} f^\dagger_{0-\sigma} f_{0-\sigma} >>_z &= < f^\dagger_{0-\sigma} f_{0-\sigma} > \\ &+ V \sum_{\vec{k}} (<< c_{\vec{k}\sigma} f^\dagger_{0-\sigma} f_{0-\sigma} | f^\dagger_{0\sigma} f^\dagger_{0-\sigma} f_{0-\sigma} >>_z \\ - << f_{0\sigma} c^\dagger_{\vec{k}-\sigma} f_{0-\sigma} | f^\dagger_{0\sigma} f^\dagger_{0-\sigma} f_{0-\sigma} >>_z &+ << f_{0\sigma} f^\dagger_{0-\sigma} c_{\vec{k}-\sigma} | f^\dagger_{0\sigma} f^\dagger_{0-\sigma} f_{0-\sigma} >>_z) \end{aligned} \qquad (11)$$

The three higher order Green functions on the right hand side of (11) vanish for $V = 0$ and are in lowest order linear in V. Because of the additional prefactor V in (11) the total expresion is of order V^2. To be exact up to order V^2 it is, therefore, justified to replace these three GFs by their lowest order contribution, which can

be easily calculated, either by a further application of the equations of motion or in finite order perturbation theory with respect to V. The result is

$$\begin{aligned}<< f_{0\sigma} f^\dagger_{0-\sigma} c_{\vec{k}-\sigma} | f^\dagger_{0\sigma} f^\dagger_{0-\sigma} f_{0-\sigma} >>_z &= \frac{V}{\epsilon_{\vec{k}} - E_{0-\sigma} - U} \\ \times \Bigg[\frac{< f^\dagger_{0\sigma} f_{0\sigma} > f(\epsilon_{\vec{k}}) - < f^\dagger_{0\sigma} f_{0\sigma} > f(E_{0-\sigma} + U) + < f^\dagger_{0-\sigma} f_{0-\sigma} > (1 - f(\epsilon_{\vec{k}}))}{z - \epsilon_{\vec{k}} - E_{0\sigma} + E_{0-\sigma}} \\ - \frac{< f^\dagger_{0-\sigma} f_{0-\sigma} > [1 - f(\epsilon_{\vec{k}})]}{z - E_{0\sigma} - U} \Bigg] &+ O(V^3) \end{aligned} \qquad (12)$$

$$\begin{aligned}<< f_{0\sigma} c^\dagger_{\vec{k}-\sigma} f_{0-\sigma} | f^\dagger_{0\sigma} f^\dagger_{0-\sigma} f_{0-\sigma} >>_z &= \frac{V}{\epsilon_{\vec{k}} - E_{0-\sigma}} \\ \times \Bigg[\frac{(1 - < f^\dagger_{0\sigma} f_{0\sigma} >)[f(\epsilon_{\vec{k}}) - f(E_{0-\sigma})] + [1 - f(\epsilon_{\vec{k}})] < f^\dagger_{0-\sigma} f_{0-\sigma} >}{z + \epsilon_{\vec{k}} - E_{0\sigma} - E_{0-\sigma} - U} \\ - \frac{< f^\dagger_{0-\sigma} f_{0-\sigma} > [1 - f(\epsilon_{\vec{k}})]}{z - E_{0\sigma} - U} \Bigg] &+ O(V^3) \end{aligned} \qquad (13)$$

$$\begin{aligned}&<< c^\dagger_{\vec{k}-\sigma} f_{0\sigma} f_{0-\sigma} | f^\dagger_{0\sigma} f^\dagger_{0-\sigma} f_{0-\sigma} >>_z \\ &= V^2 \frac{< f^\dagger_{0-\sigma} f_{0-\sigma} >}{(z - E_{0\sigma} - U)(z - \epsilon_{\vec{k}})} + O(V^3) \end{aligned} \qquad (14)$$

Simply inserting Eqs.(12 - 14) into (11) one would obtain a finite order V^2 perturbation expansion of the selfenergy or one-particle Green function; of course, infinite order resummations are desirable to obtain a selfconsistent approximation. In general, there are several possibilities to incorporate selfconsistency, but most of these possibilities lead once more to an approximation being exact up to order V^2 but not reproducing the weak-coupling limit, i.e. one obtains solutions of a similar or equivalent structure as the approximations of Ref. [32, 34], for instance. As far as we can see there is only one way to replace the Green functions on the right hand side of (11) so that also the SOPT is contained and recovered by the resulting expressions, and this approximation reads:

$$\begin{aligned}<< f_{0\sigma} f^\dagger_{0-\sigma} c_{\vec{k}-\sigma} | f^\dagger_{0\sigma} f^\dagger_{0-\sigma} f_{0-\sigma} >>_z &= \frac{1}{< f^\dagger_{0\sigma} f_{0\sigma} >< f^\dagger_{0\sigma} f_{0\sigma} f^\dagger_{0-\sigma} f_{0-\sigma} >} \\ \left(-\frac{1}{\pi}\right)^3 \int_{-\infty}^{\infty} dE_1 \int_{-\infty}^{\infty} dE_2 \int_{-\infty}^{\infty} dE_3 &\frac{[f(E_1) - f(E_3)] f(E_2) + f(E_3)[1 - f(E_1)]}{z - E_1 - E_2 + E_3} \\ Im << f_{0\sigma} | f^\dagger_{0-\sigma} f_{0-\sigma} f^\dagger_{0\sigma} >>_{E_1 + i0^+} &\; Im << c_{\vec{k}-\sigma} | f^\dagger_{0\sigma} f_{0\sigma} f^\dagger_{0-\sigma} >>_{E_2 + i0^+} \\ \times Im << f_{0-\sigma} f^\dagger_{0\sigma} f_{0\sigma} | f^\dagger_{0-\sigma} >>_{E_3 + i0^+} &+ \frac{< f^\dagger_{0\sigma} c_{\vec{k}-\sigma} f^\dagger_{0\sigma} f_{0\sigma} >}{< f^\dagger_{0\sigma} f_{0\sigma} >} << f_{0\sigma} f^\dagger_{0-\sigma} f_{0-\sigma} | f^\dagger_{0\sigma} >> \end{aligned} \qquad (15)$$

and an analogous equation for the GF $<< f_{0\sigma} c^{\dagger}_{k-\sigma} f_{0-\sigma} | f^{\dagger}_{0-\sigma} f_{0-\sigma} f^{\dagger}_{0\sigma} >>$:

$$<< f_{0\sigma} c^{\dagger}_{k-\sigma} f_{0-\sigma} | f^{\dagger}_{0-\sigma} f_{0-\sigma} f^{\dagger}_{0\sigma} >>_z = \left(-\frac{1}{\pi}\right)^3 \int_{-\infty}^{\infty} dE_1 \int_{-\infty}^{\infty} dE_2 \int_{-\infty}^{\infty} dE_3$$
$$\times \frac{(f(E_1) - f(E_3))f(E_2) + f(E_3)(1 - f(E_1))}{z - E_1 - E_2 + E_3}$$
$$\times Im << f_{0\sigma} | f_{0-\sigma} f^{\dagger}_{0-\sigma} f^{\dagger}_{0\sigma} >>_{E_1+i0^+} \; Im << f_{0-\sigma} | f^{\dagger}_{0\sigma} f_{0\sigma} f^{\dagger}_{0-\sigma} >>_{E_2+i0^+}$$
$$\times Im << f_{0-\sigma} f_{0\sigma} f^{\dagger}_{0\sigma} | c^{\dagger}_{k-\sigma} >>_{E_3+i0^+}$$
$$\frac{1}{< f^{\dagger}_{0\sigma} f_{0\sigma} f^{\dagger}_{0-\sigma} f_{0-\sigma} > (1 - < f^{\dagger}_{0\sigma} f_{0\sigma} >)} \left[\frac{< f^{\dagger}_{0-\sigma} f_{0-\sigma} >}{< f^{\dagger}_{0\sigma} f_{0\sigma} > - < f^{\dagger}_{0\sigma} f_{0\sigma} f^{\dagger}_{0-\sigma} f_{0-\sigma} >} - 1 \right]$$
$$+ \frac{< f_{0\sigma} f^{\dagger}_{0\sigma} c^{\dagger}_{k-\sigma} f_{0-\sigma} >}{1 - < f^{\dagger}_{0\sigma} f_{0\sigma} >} << f_{0\sigma} f^{\dagger}_{0-\sigma} f_{0-\sigma} | f^{\dagger}_{0\sigma} >> \quad (16)$$

and

$$(z - \epsilon_k) << c_{k\sigma} f^{\dagger}_{0-\sigma} f_{0-\sigma} | f^{\dagger}_{0\sigma} f^{\dagger}_{0-\sigma} f_{0-\sigma} >>_z = V << f_{0\sigma} f^{\dagger}_{0-\sigma} f_{0-\sigma} | f^{\dagger}_{0\sigma} f^{\dagger}_{0-\sigma} f_{0-\sigma} >>_z \quad (17)$$

In the limit of small U the theorem of Wick can be applied to the equation and the standard perturbation theory (8) up to second order in U is reproduced. In lowest order in V we insert the atomic Green's function ($V = 0$) on the right hand side of (15 - 17) and we recover (12 - 14). Therefore, these replacements (15 - 17) lead to an expression for the selfenergy of the SIAM, which is exact at least up to order U^2 in a weak coupling expansion and up to order V^2 in a strong coupling expansion. The explicit calculations within this treatment are of similar complexity as those of selfconsistent SOPT calculations, because similar energy integrals have to be evaluated only that the spectral functions of higher order instead of one-particle Green functions occur.

In summary, a new advanced many-body dynamical solution for SIAM has been developped, which recovers the exactly solvable limits $V = 0$ and $U = 0$ (5) and which is even more at least correct up to order V^2 in a strong-coupling expansion and simultaneously up to order U^2 in a weak-coupling expansion. A more detailed discussion and consideration of this new approach for the construction of a self-consistent solution for the SIAM as well as results of numerical calculations will be presented elsewhere soon.

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