EUROPHYSICS LETTERS 10 April 1996

Europhys. Lett., **34** (2), pp. 133-138 (1996)

New interpolative treatment of the single-impurity Anderson model

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(received 28 August 1995; accepted in final form 23 February 1996)

PACS. 67.40Db – Quantum statistical theory; ground state, elementary excitations.
PACS. 71.28+d – Narrow-band systems; heavy-fermion solids; intermediate-valence solids.
PACS. 75.20Hr – Local moment in compounds and alloys; Kondo effect, valence fluctuations, heavy fermions.

Abstract. – The many-body quasi-particle dynamics of the single-impurity Anderson model is investigated by means of the equations of motion for the higher-order Green's functions. It is shown that an interpolating approximation, which simultaneously reproduces the weak-coupling limit up to second order in the interaction strength U and the strong-coupling limit up to second order in the hybridization V (and thus also fulfils the atomic limit) can be formulated self-consistently.

The study of strongly correlated electrons in solids is one of the most fascinating subjects in solid-state physics [1]. The principal importance of this problem is related to the dual character of electrons in transition metal oxides, intermediate-valence solids, heavy fermions, high-T_c superconductors, etc. In these materials electrons exhibit both localized and delocalized features [2], [3]. The basic models to describe correlated electron systems are the single-impurity Anderson model (SIAM) [4] and the Hubbard model (HM) [5], which exhibit the key physical feature, *i.e.* the competition between kinetic-energy (itinerant) and potential-energy (localized) effects (cf. ref. [6]). In spite of many theoretical efforts a satisfactory solution of the dynamical problem is still missing. The Bethe-ansatz solution of the SIAM [7], [8] allows for the determination of the ground-state and thermodynamic static properties, but it does not allow for a determination of the dynamical properties. For their understanding the development of improved and reliable approximations is still justified and necessary, and a new interpolating approximation is proposed in the present paper. We will show that a self-consistent (SC) approximation for the SIAM can be formulated which reproduces all relevant exactly solvable limits and interpolates between the strong- and the weak-coupling limit. The Hamiltonian of

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the SIAM can be written in the form

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\sigma} E_{\sigma} n_{\sigma} + \frac{U}{2} \sum_{\sigma} n_{\sigma} n_{-\sigma} + \sum_{\mathbf{k}\sigma} V_{\sigma} \left(c^{\dagger}_{\mathbf{k}\sigma} f_{\sigma} + f^{\dagger}_{\sigma} c_{\mathbf{k}\sigma} \right), \tag{1}$$

where $c^{\dagger}_{\mathbf{k}\sigma}$ and $f^{\dagger}_{\sigma}$ are the creation operators for conduction and localized electrons and $n_{\sigma} = f^{\dagger}_{\sigma} f_{\sigma}$. $\epsilon_{\mathbf{k}}$ is the conduction electron dispersion, E_{σ} is the localized f electron energy level and U is the intra-atomic Coulomb interaction at the impurity site. V_{σ} represents the s-f hybridization.

We start by considering the equations of motion (EQM) for the Fourier-transformed Green's function (GF),

$$G_{\sigma}(z) = \langle\langle f_{\sigma} | f^{\dagger}_{\sigma} \rangle\rangle_z = -i \int_0^{\infty} \mathrm{d}t \exp[izt] \langle \{ f_{\sigma}(t), f^{\dagger}_{\sigma}(0) \} \rangle :,$$

$$(z - E_{\sigma} - \Delta_{\sigma}) \langle\langle f_{\sigma} | f^{\dagger}_{\sigma} \rangle\rangle_z = 1 + U \langle\langle f_{\sigma} n_{-\sigma} | f^{\dagger}_{\sigma} \rangle\rangle_z = 1 + \Sigma_{\sigma}(z) \langle\langle f_{\sigma} | f^{\dagger}_{\sigma} \rangle\rangle_z,$$

where $\Sigma_{\sigma}(z)$ is the one-particle self-energy and $\Delta_{\sigma}(z) = \sum_{\mathbf{k}} |V_{\sigma}|^2 / (z - \epsilon_{\mathbf{k}})$.

We want to develop an "interpolating" solution for the SIAM, *i.e.* a solution which is applicable in both the weak-coupling limit (and thus the exactly solvable band limit) and the strong-coupling limit (and thus the atomic limit). The simplest approximative "interpolating" solution has the form [9], [10]

$$G_{\sigma}(z) = \frac{1 - \bar{n}_{-\sigma}}{z - E_{\sigma} - \Delta_{\sigma}(z)} + \frac{\bar{n}_{-\sigma}}{z - E_{\sigma} - \Delta_{\sigma}(z) - U}. \tag{2}$$

Here $\bar{n}_{\sigma}$ denotes the occupation number of f electrons with spin σ. This is just the analogue of the Hubbard-III approximation [11] for the SIAM. As for the HM, however, Fermi-liquid (FL) properties and the Friedel sum rule, which hold for the SIAM [12] at least order by order within the U-perturbation theory, are violated within this simple approximation.

An approximation, which automatically fulfils FL properties and sum rules, is provided by the SC second-order U-perturbation treatment (SOPT) and is given by

$$\Sigma_{\sigma}(i\omega_n) = U \bar{n}_{-\sigma} - \left(\frac{U}{\beta} \right)^2 \sum_{\omega_1, \nu} G_{\sigma}(i\omega_n + i\nu) G_{-\sigma}(i\omega_1 - i\nu) G_{-\sigma}(i\omega_1). \tag{3}$$

Here $\omega_1(\nu)$ denote odd (even) Matsubara frequencies and $\beta = 1/k_{\mathrm{B}}T$. One of our goals is to find some way to incorporate this SOPT into an interpolating dynamical solution of the SIAM. This means that the approximation for the self-energy shall be correct up to order U^2 perturbationally around the band limit $U = 0$ and also the atomic limit $V = 0$ shall be fulfilled. This is the case for the SOPT around the Hartree-Fock solution [13], but only for the symmetric SIAM. For the general situation (position of the Fermi level relative to E_{σ} and $E_{\sigma} + U$) a heuristic semi-empirical approach for constructing such an approximation has been presented for the SIAM in ref. [14] and for the HM in ref. [15]-[17]; the Edwards-Hertz-approximation [15] (EHA) can also easily be applied to the SIAM. Our intention is to take into account the SC-SOPT. Furthermore, in contrast to ref. [13]-[15] the approximation shall not only fulfil the atomic limit $V = 0$, but it shall be correct up to order V^2 in a strong-coupling expansion around the atomic limit. The SC inclusion of contributions in second- (and fourth-) order perturbation theory around the atomic limit is, in particular, important to properly account for the Kondo effect within the SIAM (Kondo temperature scale) and to reproduce the correct antiferromagnetic behaviour (equivalence to the t-J model) in the strong-coupling limit of the HM [17].

During the last decades several different refined many-body techniques have been applied to the SIAM [18]-[33] 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 V. When applied to the calculation of static properties many of these treatments, in particular the "non-crossing approximation" (NCA) [20]-[22] and its improvements [23]-[25], give results in remarkably good agreement with the exact Bethe-ansatz results [2]. But for the many-body dynamics the results of most of these approximations are not fully satisfactory, in particular as FL properties and sum rules are violated. Furthermore, when applied to the finite-U SIAM none of these approximation schemes [18]-[33] reproduce the SOPT. Qualitatively the dynamical properties of the SIAM are known from the NCA and from numerical results obtained by the numerical renormalization group method [34] and by quantum Monte Carlo methods [35]. These available numerical results will allow for a comparison with the results of the improved analytical approach so that the quality of the approximation may be judged.

To construct this interpolating approximation for the SIAM fulfilling all desired properties mentioned above we start from the EQM for the higher-order GF $\langle\langle f_\sigma n_{-\sigma}|f_\sigma^\dagger\rangle\rangle_z$:

$$(z - E_\sigma - \Delta_\sigma - U)\langle\langle f_\sigma n_{-\sigma}|f_\sigma^\dagger\rangle\rangle_z = \bar{n}_{-\sigma} - U\langle\langle f_\sigma f_{-\sigma} f_{-\sigma}^\dagger|f_\sigma^\dagger n_{-\sigma}\rangle\rangle_z\,.$$

With $[G_\sigma^{(0)}(z)]^{-1} = z - E_\sigma - \Delta_\sigma$ and the SC summation $[G_\sigma^{(0)}(z)]^{-1}G_\sigma(z) = 1 + \Sigma_\sigma(z)G_\sigma(z)$, we derive from this EQM the following exact relation:

$$\Sigma_\sigma(z) = \frac{U\bar{n}_{-\sigma} + U^2\mathcal{S}(z)\frac{G_\sigma(z)}{1+\Sigma_\sigma(z)G_\sigma(z)}}{1 - (U - \Sigma_\sigma(z))G_\sigma(z)}\,, \tag{4}$$

with the definition $\langle\langle f_\sigma f_{-\sigma} f_{-\sigma}^\dagger|f_\sigma^\dagger n_{-\sigma}\rangle\rangle_z = -\mathcal{S}(z)\frac{G_\sigma(z)}{1+\Sigma_\sigma(z)G_\sigma(z)}$.

Applying the EQM to the higher-order GF $\langle\langle f_\sigma f_{-\sigma} f_{-\sigma}^\dagger|f_\sigma^\dagger n_{-\sigma}\rangle\rangle_z$ one obtains for the function $\mathcal{S}(z)$ the exact equation

$$\mathcal{S}(z) = V_{-\sigma}\sum_{\mathbf{k}}\left\{G_{1\sigma}(\underline{\mathbf{k}}) - G_{2\sigma}(\underline{\mathbf{k}}) + \frac{V_\sigma}{z - \epsilon_{\mathbf{k}}}\left[G_{3\sigma}(\underline{\mathbf{k}}) - G_{4\sigma}(\underline{\mathbf{k}})\right]\right\}, \tag{5}$$

with $\underline{\mathbf{k}} = (\mathbf{k}, z)$ and $G_{1\sigma}(\underline{\mathbf{k}}) = \langle\langle f_\sigma f_{-\sigma}^\dagger c_{\mathbf{k}-\sigma}|f_\sigma^\dagger n_{-\sigma}\rangle\rangle_z$, $G_{2\sigma}(\underline{\mathbf{k}}) = \langle\langle f_\sigma c_{\mathbf{k}-\sigma}^\dagger f_{-\sigma}|f_\sigma^\dagger n_{-\sigma}\rangle\rangle_z$, $G_{3\sigma}(\underline{\mathbf{k}}) = \sum_{\mathbf{q}}\langle\langle c_{\mathbf{k}\sigma} f_{-\sigma} c_{\mathbf{q}-\sigma}^\dagger|f_\sigma^\dagger n_{-\sigma}\rangle\rangle_z$, $G_{4\sigma}(\underline{\mathbf{k}}) = \sum_{\mathbf{q}}\langle\langle c_{\mathbf{k}\sigma} c_{\mathbf{q}-\sigma} f_{-\sigma}^\dagger|f_\sigma^\dagger n_{-\sigma}\rangle\rangle_z$.

In general, there are several possibilities to incorporate SC, 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. [27], [33], for instance. To be exact up to order V^2 it is justified to replace the higher-order GFs on the right-hand side of eq. (5) by their lowest-order contributions, which are given by

$$\begin{cases} G_{1\sigma}(\underline{\mathbf{k}}) = \frac{V_{-\sigma}}{\epsilon_{\mathbf{k}} - E_{-\sigma} - U}\left[\frac{\bar{n}_\sigma[f_{\mathbf{k}} - f(E_{-\sigma}+U)] + \bar{n}_{-\sigma}[1-f_{\mathbf{k}}]}{z - \epsilon_{\mathbf{k}} - E_\sigma + E_{-\sigma}} - \frac{\bar{n}_{-\sigma}[1-f_{\mathbf{k}}]}{z - E_\sigma - U}\right] + \mathrm{O}\,(V^3), \\ G_{2\sigma}(\underline{\mathbf{k}}) = \frac{V_{-\sigma}}{\epsilon_{\mathbf{k}} - E_{-\sigma}}\left[\frac{(1-\bar{n}_\sigma)[f_{\mathbf{k}} - f(E_{-\sigma})] + [1-f_{\mathbf{k}}]\bar{n}_{-\sigma}}{z + \epsilon_{\mathbf{k}} - E_\sigma - E_{-\sigma} - U} - \frac{\bar{n}_{-\sigma}[1-f_{\mathbf{k}}]}{z - E_\sigma - U}\right] + \mathrm{O}\,(V^3), \\ G_{3\sigma}(\underline{\mathbf{k}}) = \mathrm{O}\,(V^2),\ G_{4\sigma}(\underline{\mathbf{k}}) = \mathrm{O}\,(V^2), \end{cases} \tag{6}$$

leading to a finite-order V^2 perturbation expansion of the self-energy (4).

$f(E) = \{\exp[(E-\mu)/k_\mathrm{B}T] + 1\}^{-1}$ is the Fermi function, μ the chemical potential and $f_{\mathbf{k}} = f(\epsilon_{\mathbf{k}})$.

For the higher-order Green's functions $G_{i\sigma}(\underline{\mathbf{k}})$ $(i = 1, \ldots, 4)$ one can find an approximation which reproduces the exact relations (6) in lowest order in V and is simultaneously exact in lowest order in U (when Wick's theorem is applicable). One possibility for such an approximation is given by

$$\begin{aligned} G_{1\sigma}(\underline{\mathbf{k}}) &= \frac{-\beta^{-2}}{\bar{n}_\sigma \langle n_\sigma n_{-\sigma}\rangle} \sum_{\omega_1,\nu} \langle\langle f_\sigma | n_{-\sigma} f_\sigma^\dagger \rangle\rangle_{i\omega_n + i\nu} \langle\langle c_{\mathbf{k}-\sigma} | n_\sigma f_{-\sigma}^\dagger \rangle\rangle_{i\omega_1 - i\nu} \times \\ &\times \langle\langle f_{-\sigma} n_\sigma | f_{-\sigma}^\dagger \rangle\rangle_{i\omega_1} + \frac{\langle f_{-\sigma}^\dagger c_{\mathbf{k}-\sigma} n_\sigma \rangle}{\bar{n}_\sigma} \langle\langle f_\sigma n_{-\sigma} | f_\sigma^\dagger \rangle\rangle_{i\omega_n}\,, \qquad (7) \\ G_{2\sigma}(\underline{\mathbf{k}}) &= \frac{-\beta^{-2}}{(1-\bar{n}_\sigma)\langle n_\sigma n_{-\sigma}\rangle} \sum_{\omega_1,\nu} \Bigg(\frac{\bar{n}_\sigma}{\bar{n}_\sigma - \langle n_\sigma n_{-\sigma}\rangle} \langle\langle f_\sigma | f_{-\sigma} f_{-\sigma}^\dagger f_\sigma^\dagger \rangle\rangle_{i\omega_n + i\nu} \times \\ &\times \langle\langle f_{-\sigma} | n_\sigma f_{-\sigma}^\dagger \rangle\rangle_{i\omega_1 - i\nu} - \langle\langle f_\sigma | n_{-\sigma} f_\sigma^\dagger \rangle\rangle_{i\omega_n + i\nu} \langle\langle f_{-\sigma} | f_\sigma f_\sigma^\dagger f_{-\sigma}^\dagger \rangle\rangle_{i\omega_1 - i\nu} \Bigg) \times \\ &\times \langle\langle f_{-\sigma} f_\sigma f_\sigma^\dagger | c_{\mathbf{k}-\sigma}^\dagger \rangle\rangle_{i\omega_1} + \frac{\langle f_\sigma f_\sigma^\dagger c_{\mathbf{k}-\sigma}^\dagger f_{-\sigma} \rangle}{1-\bar{n_\sigma}} \langle\langle f_\sigma n_{-\sigma} | f_\sigma^\dagger \rangle\rangle_{i\omega_n}\,, \qquad (8) \end{aligned}$$

and the GF $G_{3\sigma}, G_{4\sigma}$ are decoupled according to the theorem of Wick. Since the approximation does not violate the theorem of Wick for small U, it automatically satisfies the SOPT, *i.e.* expanding eq. (4) for small U up to second order in U leads to the SOPT for the self-energy. Also the V^2-limit is not violated since the GF $G_{3\sigma}, G_{4\sigma}$ are themselves proportional to V^2, leading in eq. (5) to V^4 terms. Therefore, our approximation leads to an expression for the self-energy of the SIAM, which is exact at least up to order U^2 in a weak-coupling expansion and up to order V^2 in a strong-coupling expansion. The structure of the chosen approximation (7), (8) and of the decoupling for the GF $G_{3\sigma}, G_{4\sigma}$ according to the theorem of Wick has a similar analytical structure as the SOPT (which can be calculated numerically very fast and accurately, [36]). Hence the explicit numerical calculations within this treatment are of the same order of complexity as those of the SC-SOPT calculations.

Notice that in principle it is possible to systematically improve the above approximation. Since the SC summation (4), (5) is formally exact, the next step would be the similar construction of an approximation for the GFs $G_{3\sigma}, G_{4\sigma}$ (and for GFs of a similar structure occurring in a further application of the EQM to the GFs $G_{1\sigma}, G_{2\sigma}$) being exact in order V^2 and simultaneously satisfying the theorem of Wick; as the GFs $G_{3\sigma}$ etc. have already a prefactor V^2 in (5), this leads to an approximation for $\mathcal{S}$ and thus the self-energy $\Sigma_\sigma(z)$ being exact up to order V^4 in the strong-coupling limit and simultaneously in order U^2 in the weak-coupling limit. Furthermore, already from the structure of the exact equation (4) it is clear that our new approximation can be considered as a systematic improvement of the Hubbard-III-approximation (2), which is known to be reasonable concerning the high-frequency behaviour of the dynamical quantities and concerning the reproduction of the metal-insulator transition in the HM. The new approach goes beyond the Hubbard-III-approximation including all self-energy contributions in order U^2 and thus reproducing the SOPT. This is important to fulfil the FL properties at least for small U, and in this respect the approach should be as good as the recently investigated EHA [15], [16] and related attempts [14], [37]. On the other hand, the new approach is also exact up to order V^2 and is, therefore, as good as standard EQM decouling procedures [26]-[28] are, which qualitatively describe important items like Kondo peak, Kondo temperature scale, etc. Finally the approach is not a completely uncontrolled approximation, as it is exact up to certain orders (V^2, U^2) of systematic perturbation theory. It is, however, as any SC approximate treatment is, uncontrolled in the way it takes into account infinite-order resummations of arbitrary order in U and V by the SC requirement,

which is unavoidable to reproduce both limits.

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

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One of the authors (ALK) is grateful to Deutsche Forschungsgemeinschaft for financial support and to University of Bremen for a kind hospitality.

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