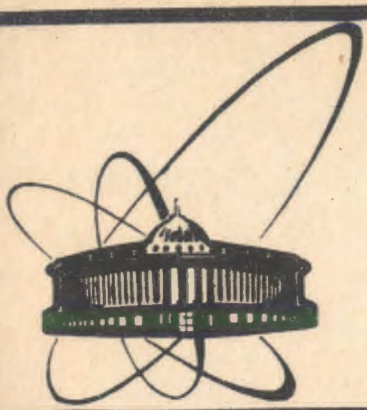

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CORRELATION EFFECTS IN THE SINGLE-IMPURITY ANDERSON MODEL. WEAK AND STRONG COULOMB INTERACTION

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1. INTRODUCTION

The single-impurity Anderson model (SIAM) has been proposed many years ago[1] to describe highly dilute random alloys[2,3]. In practice, this model is used to imitate other systems too. For example, more recently this model has been widely used to describe mixed valence and heavy fermion systems [4-7]. Although it is a simplified model, nevertheless it contains most of the relevant physics and a great deal of interesting works has been done on it [2-7]. But it still remains only partially solved. The elegant Bethe-Anzatz technique as applied to the reduced Anderson model[3] leads to the exact static solution of SIAM only. The generalization of this approach for realistic k^2 electron spectrum has not been done yet.

In the past years many efforts have been made to calculate dynamical properties of SIAM using various advanced methods of many-body theory[4-15]. Unfortunately, the proposed solutions are, as a rule, limited in several ways; they are valid for a rather narrow intervals of relevant parameters. Moreover, no general concept for construction of the interpolating dynamical solution of SIAM has been proposed. In such situation the unified self-consistent approach, which permits to obtain a solution interpolating between weak and strong correlation limits, is highly desirable.

In this paper we present a unified self-consistent calculation of the one-electron Green function (GF) which gives the correct results both for the weak and the strong Coulomb correlations. The approach we suggest is founded on the same type of concept which has proved to be valuable for Hubbard model[16-17] and which has been suggested as essential for various many-body systems with complex spectrum and strong interaction[16-21]. We believe that the solutions which are derived below bear the real physics of SIAM.

2. OUTLINE OF THE METHOD

The irreducible GF(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 GF's (or the irreducible parts of the operators, out of which the GF is constructed) in terms of which it is possible, without recourse to a truncation of the hierarchy of equations for the GF's, to write down the exact Dyson equation and to obtain an exact analytical representation for 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 separation and identification of elastic scattering effects and inelastic ones. The irreducible GF's are so defined 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 and puts them into the generalized mean-field GF.It is worth to emphasize that, in general, the mean-field renormalizations can exhibit quite nontrivial structure. To obtain this structure correctly, one must construct the full GF built of the complete algebra of relevant operators and develop a special projection procedure for higher-order GF's in accordance with the algebra found. The most important feature of this approach is a very nontrivial structure of the mean-field renormalizations as found in cases of the Hubbard model in the strong correlation limit /16/ and the magnetic polaron problem at finite temperatures and an arbitrary value of s-f exchange /19,20/. It is important to note that there is a possibility of generalizing the scheme described above introducing IGF's for higher-order equation of motion /21/.

3. SIAM. WEAK CORRELATION

Let us consider the standard one-impurity Anderson Hamiltonian /1/

$$H = \sum_{k\sigma} \epsilon_k c^+_{k\sigma} c_{k\sigma} + \epsilon_d \sum_\sigma d^+_{0\sigma} d_{0\sigma} + U/2 \sum_\sigma n^d_{0\sigma} n^d_{0-\sigma} + \\ + \sum_{k\sigma} V_k (c^+_{k\sigma} d_{0\sigma} + d^+_{0\sigma} c_{k\sigma}). \qquad (1)$$

This is the basic Hamiltonian which will be discussed here. The simplest way of dealing with (1) is to apply the Hartree-Fock (HF) theory /1/. But, as it was pointed in review paper /3/, it is a fairly rough approximation which has no region of applicability. Nevertheless, from the formal point of view we consider that the validity region of it is limited to weak correlation ($U \to 0$) only. In this limit, due to the mixing of d and s states, the resonance level exhibits a finite width. We will give below the IGF calculations for $U \to 0$.

For calculation of the electronic quasiparticle spectrum of the model described by Hamiltonian (1) let us consider the equations of motion for one-electron GF's

$$\ll c_{k\sigma}(t)\, c^+_{k\sigma}(t') \gg = -i\theta(t-t') \langle [\, c_{k\sigma}(t), c^+_{k\sigma}(t')\,]_+ \rangle, \qquad (2)$$

$$\ll d_{0\sigma}(t)\, d^+_{0\sigma}(t') \gg = -i\theta(t-t') \langle [\, d_{0\sigma}(t), d^+_{0\sigma}(t')\,]_+ \rangle. \qquad (3)$$

Because of c-d coupling GF's (2) and (3) are elements of the matrix GF

$$G(\omega) = \begin{bmatrix} \ll c_{k\sigma} | c^+_{k\sigma} \gg_\omega & \ll c_{k\sigma} | d^+_{0\sigma} \gg_\omega \\ \ll d_{0\sigma} | c^+_{k\sigma} \gg_\omega & \ll d_{0\sigma} | d^+_{0\sigma} \gg_\omega \end{bmatrix} \qquad (4)$$

Performing first time t differentiation of (4) and introducing the irreducible GF by definition /16,17/

$$^{ir}\ll d_{0\sigma} n_{0-\sigma} | d^+_{0\sigma} \gg = \ll d_{0\sigma} n_{0-\sigma} | d^+_{0\sigma} \gg - \langle n_{0-\sigma} \rangle \ll d_{0\sigma} | d^+_{0\sigma} \gg \qquad (5)$$

we obtain the following equation in matrix form

$$\sum_p \hat{\Phi}_p(\omega) \cdot \hat{G}(\omega, p) = \hat{1} + U \hat{D}^{ir}(\omega), \qquad (6)$$

where all definitions are rather evident. In order to calculate the higher-order GF on the r.h.s. of (6) we have to write the equation of motion obtained by means of differentiation with respect to the second time variable t'. Definition (5) allows one to remove the inhomogeneous term in this equation. If one introduces irreducible parts for the r.h.s. operators by analogy with expression (5), the equation of motion (6) can be exactly rewritten in the form of the DYSON equation

$$\hat{G} = \hat{G}^0 + \hat{G}^0 \hat{M} \hat{G}. \qquad (7)$$

The generalized mean-field GF $\hat{G}^0$ satisfies equation

$$\sum_p \hat{\Phi}_p(\omega) \hat{G}^0(\omega, p) = \hat{1}. \qquad (8)$$

The explicit solution of (8) for diagonal elements is

$$\ll c_{k\sigma} | c^{+}_{k\sigma} \gg^{0}_{\omega} = \{\omega - \epsilon_k - \frac{|V_k|^2}{\omega - \epsilon_d - Un_{-\sigma} - \sum_p \frac{|V_p|^2}{\omega - \epsilon_p}}\}^{-1} \quad (9)$$

$$\ll d_{0\sigma} | d^{+}_{0\sigma} \gg^{0}_{\omega} = \{\omega - \epsilon_d - Un_{-\sigma} - \sum_p \frac{|V_p|^2}{\omega - \epsilon_p}\}^{-1}, \quad (10)$$

these expressions coincide with Anderson's HF result /1/ and in the limit $U = 0$ lead to exact results for GFs.

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

$$\hat{M} = \begin{bmatrix} 0 & 0 \\ 0 & M^{\sigma}_{00} \end{bmatrix}, \quad (11)$$

where

$$M^{\sigma}_{00} = U^2 \ll^{ir} d_{0\sigma} n_{0-\sigma} | d^{+}_{0\sigma} n_{0-\sigma} \gg^{ir}_{\omega}. \quad (12)$$

Thus, by introducing irreducible parts of GF (or the irreducible parts of the operators, out of which the GF is constructed) the equations of motion for the GF(4) were exactly transformed into a Dyson equation (7) with an exact representation of the self-energy operator, expressed in terms of higher order GF. It should be emphasized that for weak correlation case, $U \to 0$, the functional of the mean-field renormalization can be represented in terms of mean densities of electrons (see Eq.(5)).

The formal solution of Dyson equation (7) can be written as

$$G = \{(G^0)^{-1} - M\}^{-1}. \quad (13)$$

From (13) one immediately obtains

$$\ll d_{0\sigma} | d^{+}_{0\sigma} \gg_{\omega} = \{\omega - \epsilon_d - Un_{-\sigma} - M^{\sigma}_{00} - \sum_p \frac{|V_p|^2}{\omega - \epsilon_p}\}^{-1},$$

$$\ll c_{k\sigma} | c^{+}_{k\sigma} \gg_{\omega} = \{\omega - \epsilon_k - \frac{|V_k|^2}{\omega - \epsilon_d - Un_{-\sigma} - M^{\sigma}_{00}}\}. \quad (14)$$

In order to calculate the self-energy operator in a self-consistent way, we have to express it approximately by lower order GF's. Let us start in analogy with Hubbard model with a pair-type approximation

$$M^{\sigma}_{00}(\omega) \approx U^2 \int_{-\infty}^{\infty} \frac{d\omega_1 d\omega_2 d\omega_3}{\omega + \omega_1 - \omega_2 - \omega_3} \{ n(\omega_1)[1 - n(\omega_2) - n(\omega_3)] + n(\omega_2) n(\omega_3) \} g_{0-\sigma}(\omega_1) g_{0\sigma}(\omega_2) g_{0-\sigma}(\omega_3), \quad (15)$$

where

$$g_{0\sigma} = -\frac{1}{\pi} \operatorname{Im} \ll d_{0\sigma} | d^{+}_{0\sigma} \gg.$$

If we take for the first iteration step

$$g_{0\sigma} \sim \delta(\omega - \epsilon_d - Un_{-\sigma}), \quad (16)$$

we immediately obtain $M^{\sigma}_{00} = 0$. This result reflects the fact that only one impurity site is present. For periodic Anderson model the pair approximation (15) should work quite well.

Let us try (again in analogy with the Hubbard model /16/) another type of approximation for M. Owing to the well-known spectral theorem the GF in the r.h.s. of (12) can be expressed in terms of correlation functions. The approximation which we will use now reflects the interference between the one-particle branch and the collective one:

$$\begin{aligned} &\langle d^{+}_{0-\sigma} d_{0-\sigma} d^{+}_{0\sigma} d_{0\sigma}(t)\, d^{+}_{0-\sigma}(t)\, d_{0-\sigma}(t) \rangle \approx \\ &\approx \langle n_{0-\sigma} n_{0-\sigma}(t) \rangle \langle d^{+}_{0\sigma} d_{0\sigma}(t) \rangle + \\ &+ \langle d^{+}_{0\sigma} d_{0-\sigma} d^{+}_{0-\sigma}(t)\, d_{0\sigma}(t) \rangle \langle d^{+}_{0-\sigma} d_{0-\sigma}(t) \rangle + \\ &+ \langle d^{+}_{0\sigma} d^{+}_{0-\sigma} d_{0-\sigma}(t)\, d_{0\sigma}(t) \rangle \langle d_{0-\sigma} d^{+}_{0-\sigma}(t) \rangle . \end{aligned} \quad (17)$$

If we retain only the first term in (17) (cf. /12/) and make use of the same first iteration as (16), we obtain for the self-energy operator

$$M_{\sigma}(\omega) = U^2 \frac{1 - n(\epsilon_d - Un_{-\sigma})}{\omega - \epsilon_d - Un_{-\sigma}} \langle n_{0-\sigma} n_{0-\sigma} \rangle. \quad (18)$$

It is very interesting that when retaining the second term in (17) we obtain

$$\ll d_{0\uparrow} | d^{+}_{0\uparrow} \gg_{\omega} = \{\omega - \epsilon_d - U n_{\downarrow} - M^{\uparrow}_{00}(\omega) - \sum_p \frac{|V_p|^2}{\omega - \epsilon_p}\}^{-1}, \tag{19}$$

$$\ll d_{0\downarrow} | d^{+}_{0\downarrow} \gg_{\omega} = \{\omega - \epsilon_d - U n_{\uparrow} - M^{\downarrow}_{00}(\omega) - \sum_p \frac{|V_p|^2}{\omega - \epsilon_p}\}^{-1}, \tag{20}$$

where

$$M^{\sigma}_{00}(\omega) = U^2 \int_{-\infty}^{\infty} d\omega_1 d\omega_2 \frac{1 + N(\omega_1) - n(\omega_2)}{\omega - \omega_1 - \omega_2} \{-\frac{1}{\pi} \mathrm{Im} \ll S^{\mp}_0 | S^{\pm}_0 \gg_{\omega_1}\} \times$$

$$\times \{-\frac{1}{\pi} \mathrm{Im} \ll d_{0\sigma} | d^{+}_{0\sigma} \gg_{\omega_2}\} \tag{21}$$

with $S^{+}_0 = d^{+}_{0\uparrow} d_{0\downarrow}$; $S^{-}_0 = d^{+}_{0\downarrow} d_{0\uparrow}$ or, in more convenient form, (cf.[12])

$$M^{\sigma}_{00}(\omega) = U^2 \int d\omega_1 \{\coth \frac{\omega - \omega_1}{2T} + \tanh \frac{\omega_1}{2T}\} \times$$

$$\times \{-\frac{1}{\pi} \mathrm{Im} \chi^{\mp\pm}_{00}(\omega - \omega_1)\} g_{0\sigma}(\omega_1). \tag{22}$$

The essential feature of this approximation is connected with the fact that spin up and spin down electrons are correlated when they occupy the impurity level. So this really improves the HF theory in which just these correlations are missed. The scattering of the d-electron with the band electron causes the impurity level to be shifted and broadened. But by including the correlation effects for the weak correlation case we obtain additional shift and broadening due to electron-electron inelastic scattering processes. This, of course, leads to small corrections for shift and width and influences mainly on the line form of spectral density. The role of electron-electron correlation becomes much more crucial for the case of strong correlation. In the region where U is very large, but finite, the theory faces the most serious difficulties[14].

4. SIAM. STRONG CORRELATION

To depict the behaviour of the system in the case of strong Coulomb correlations when the scattering between the band and d electrons is present we need a more sophisticated approach than one proposed in papers[8-15]. The relevant algebra of the operators used for description of the strong correlation has the similar form as for Hubbard model[16]. Let us represent matrix GF (4) in the following form

$$\hat{G}_{\sigma}(\omega) = \begin{bmatrix} \ll c_{k\sigma} | c^{+}_{k\sigma} \gg_{\omega} & \sum_{\beta} \ll c_{k\sigma} | f^{+}_{0\beta\sigma} \gg_{\omega} \\ \sum_{\alpha} \ll f_{0\alpha\sigma} | c^{+}_{k\sigma} \gg_{\omega} & \sum_{\alpha\beta} \ll f_{0\alpha\sigma} | f^{+}_{0\beta\sigma} \gg \end{bmatrix}, \tag{23}$$

where

$$f_{0\alpha,\sigma} = n^{\alpha}_{0-\sigma} d_{0\sigma} (\alpha = \pm); \quad n^{+}_{0\sigma} = n_{0\sigma}; \quad n^{-}_{0\sigma} = (1 - n_{0\sigma}). \tag{24}$$

The equation of motion for auxiliary GF $\tilde{G}$

$$\hat{\tilde{G}}_{\sigma}(\omega) = \begin{bmatrix} \ll c_{k\sigma} | c^{+}_{k\sigma} \gg_{\omega} & \ll c_{k\sigma} | f^{+}_{0+\sigma} \gg_{\omega} & \ll c_{k\sigma} | f^{+}_{0-\sigma} \gg_{\omega} \\ \ll f_{0+\sigma} | c^{+}_{k\sigma} \gg_{\omega} & \ll f_{0+\sigma} | f^{+}_{0+\sigma} \gg_{\omega} & \ll f_{0+\sigma} | f^{+}_{0-\sigma} \gg_{\omega} \\ \ll f_{0-\sigma} | c^{+}_{k\sigma} \gg_{\omega} & \ll f_{0-\sigma} | f^{+}_{0+\sigma} \gg_{\omega} & \ll f_{0-\sigma} | f^{+}_{0-\sigma} \gg_{\omega} \end{bmatrix} \tag{25}$$

in the matrix notation reads

$$\hat{E} \hat{\tilde{G}}_{\sigma}(\omega) - \hat{I} = \hat{D}, \tag{26}$$

where

$$\hat{E} = \begin{bmatrix} (\omega - \epsilon_k) & -V_k & -V_k \\ 0 & (\omega - \epsilon_d - U_+) & 0 \\ 0 & 0 & (\omega - \epsilon_d - U_-) \end{bmatrix}; \quad U_{\alpha} = \begin{cases} U, & \alpha = + \\ 0, & \alpha = - \end{cases} \tag{27}$$

and

$$\hat{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & n^{+}_{0-\sigma} & 0 \\ 0 & 0 & n^{-}_{0-\sigma} \end{bmatrix}; \quad \hat{D} = \begin{bmatrix} 0 & 0 & 0 \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{bmatrix} \tag{28}$$

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

$$D_{22} = \ll(c_{p\sigma} n_{0-\sigma} + d^{+}_{0-\sigma} c_{p-\sigma} d_{0\sigma} - c^{+}_{p-\sigma} d_{0-\sigma} d_{0\sigma}) \mid f^{+}_{0+\sigma} \gg_{\omega},$$

$$D_{33} = \ll(c_{p\sigma}(1 - n_{0-\sigma}) - d^{+}_{0-\sigma} c_{p-\sigma} d_{0\sigma} + c^{+}_{p-\sigma} d_{0-\sigma} d_{0\sigma}) \mid f^{+}_{0-\sigma} \gg_{\omega}. \qquad (29)$$

Let us introduce the matrix irreducible GF $\tilde{D}^{ir}$ in accordance with the definition given in the paper [16]

$$\hat{D}^{ir} = \hat{D} - \sum_{a} \begin{bmatrix} A^{+a} \\ A^{-a} \end{bmatrix} [\tilde{G}^{a+}_{\sigma} \quad \tilde{G}^{a-}_{\sigma}], \qquad (30)$$

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

$$< [\hat{D}^{ir}_{a\beta}, f^{+}_{0\beta\sigma}] > \equiv 0. \qquad (31)$$

The corresponding exact Dyson equation is

$$\hat{\tilde{G}} = \hat{\tilde{G}}^{0} + \hat{\tilde{G}}^{0} \hat{M} \hat{\tilde{G}}, \qquad (32)$$

where G^{0} is the generalised mean-field GF. It is very important to show the explicit form of the mean-field renormalizations

$$A^{++} = \frac{< (d^{+}_{0-\sigma} c_{p-\sigma} + c^{+}_{p-\sigma} d_{0-\sigma})(n_{0\sigma} - n_{0-\sigma}) >}{< n_{0-\sigma} >}, \qquad (33)$$

$$A^{--} = \frac{-< (d^{+}_{0-\sigma} c_{p-\sigma} + c^{+}_{p-\sigma} d_{0-\sigma})(1 + n_{0\sigma} - n_{0-\sigma}) >}{(1 - n_{0-\sigma})}, \qquad (34)$$

$$A^{-+} = -A^{++}; \quad A^{+-} = -A^{--}.$$

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

$$\ll d_{0\sigma} \mid d^{+}_{0\sigma} \gg^{0}_{\omega} = \frac{< n_{0-\sigma} >}{\omega - \epsilon_d - U_+ - \sum_p V_p A^{++}} \left(1 + \frac{\sum_p V_p A^{-+}}{\omega - \epsilon_d - U_-}\right) +$$

$$+ \frac{(1 - < n_{0-\sigma} >)}{\omega - \epsilon_d - U_- - \sum_p V_p A^{--}} \left(1 + \frac{\sum_p V_p A^{+-}}{\omega - \epsilon_d - U_+}\right). \qquad (35)$$

For the $V_p = 0$ we obtain exact atomic solution

$$F^{at} = \frac{< n_{0-\sigma} >}{\omega - \epsilon_d - U_+} + \frac{(1 - < n_{0-0} >)}{(\omega - \epsilon_d - U_-)}.$$

The conduction electron GF in this approximation reads

$$\ll c_{k\sigma} \mid c^{+}_{k\sigma} \gg^{0}_{\omega} = \{\omega - \epsilon_k - |V_k|^2 F^{at}(\omega)\}^{-1}.$$

This form of solution also gives the correct expression for $V_k = 0$. The self-energy operator has the form

$$\hat{M} = \hat{I}^{-1} \{\sum_{pq} V_p V_q \ll \hat{D}^{ir} \mid (\hat{D}^{ir})^{+} \gg\} \hat{I}^{-1}.$$

This equation is an analogue of the equation for the self-energy operator in the Hubbard model [16] so we are not going to write it explicitly here especially because of its complicated structure. But it is important to note that the self-energy operator for the periodic Anderson model is much more similar to the self-energy operator of the Hubbard model.

5. CONCLUSIONS

In summary, we have obtained the new interpolation solution - one-particle GF for the SIAM in the framework of IGF formalism. In the weak correlation case the functional of the generalized mean-fields (GMF) depends only of mean electron densities and this solution improves the HF solution [1] and allows to incorporate the correlation of the spin-up and spin-down electrons occupying the impurity level, in a self-consistent way. For the case of a strong Coulomb correlation we obtained an essentially new solution confirming the statement [16-21] that in this case the mean-field renormalization has a quite nontrivial structure and cannot be reduced to the mean density functional. The theory we suggest allows one to find explicitly the damping of quasiparticle excitations in a self-consistent way as it was demonstrated in detail here for weak correlation case. And lastly, it should be emphasized that SIAM and periodic Anderson model (PAM) will have very different structure of GMF as well as the

structure of inelastic scattering corrections due to the self-energy operator. The more detailed analysis of the obtained solution and a comparison with the solution for PAM will be published elsewhere.

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