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Analytical approximation for single-impurity Anderson model

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We propose a new renormalized strong-coupling expansion to describe the electron spectral properties of single-band Anderson impurity problem in a wide energy range. The first-order result of our scheme reproduces well the entire single-electron spectrum of correlated impurity with the Kondo-like logarithmic contributions to the self energy and the renormalization of atomic resonances due to hybridization with conduction electrons. The Friedel sum rule for a half-filled system is fulfilled. The approach is based on so-called dual transformation, so that the series is constructed in vertices of the corresponding atomic Hamiltonian problem. The atomic problem of single impurity has a degenerate ground state, so the application of the perturbation theory is not straightforward. We construct a special approach dealing with symmetry-broken ground state of the atomic problem. The renormalization ensures a convergence near the frequencies of atomic resonances. Proposed expansion contains a small parameter in the weak- and in the the strong-coupling case and interpolates well in between. Formulae for the first-order dual diagram correction are obtained analytically in the real-time domain. A generalization of this scheme to a multi-orbital case can be important for the realistic description of correlated solids.

Introduction. The problem of realistic description of spectral properties of correlated impurity in the metallic surrounding is far from solution despite of considerable progress during the past years. There are quite successful tools for large Coulomb U, particularly diagrammatic pseudoparticle approach [1]. Transport properties can be described in this limit also [2, 3]. The case of moderate U is less studied, although there is an interesting physics behind, e.g. renormalization of the multiplet structure due to hybridization with conduction band. Exact solutions by using the Bethe-ansatz are obtained for thermodynamical [4, 5] and steady-state transport [6] properties. There are numerically exact continuous-time quantum Monte Carlo calculations in imaginary time domain[7, 8]. Practical accuracy of these methods is limited by an ill-posed problem of analytical continuation to the real-frequency axis. More accurate data can be obtained within the Numerical Renormalization Group framework [9].

Two previous works should are particularly important for our paper. First, we refer to a numerical RPA-like approach [10]. All Kondo properties are described surprisingly well, if the consideration starts from a local-moment broken symmetry solution. The Abrikosov-Suhl resonance, Kondo energy scale and Friedel sum rule have been reproduced. Second, we mention the superperturbation solver [11], that is a kind of strong-coupling expansion around an exact paramagnetic solution for certain cluster. That theory performs well for a moderately low temperatures, but suffers serious problems as temperature goes to zero.

In the present paper we propose an analytical approximation for spectral properties of a single-band Anderson impurity model (SIAM) with moderate U at zero temperature. Our zero approximation is a mean-field solution constructed for a symmetry-broken state of the atomic problem. The theory utilizes an exact mapping of the SIAM to auxiliary (dual) variables [12, 13] in a real-time domain. Another important property of our method is a renormalization procedure, which allows to describe a shift of the atomic resonances due to hybridization with a conduction band. Similar to [10] and [11], our scheme provides a description of SIAM at different energy scales, including renormalization of the spectral function of the entire conduction band. This is of particular importance for the realistic description of multi-orbital correlated solids in the Dynamical Mean Field framework. On the other hand, it does not pretend to describe the physics below Kondo scale, where renormalization-group analysis is required [4, 5, 9].

Anderson impurity problem. We consider a single-band Anderson impurity problem at zero temperature with the following action (summations over spin index $\sigma = \uparrow, \downarrow$ are supposed):

$$S = S_{at} - \iint_{-\infty}^{+\infty} dt\, dt' \bar{c}_{\sigma t} \Delta(t-t') c_{\sigma t'},$$
$$S_{at} = \int_{-\infty}^{+\infty} dt \left(i\bar{c}_{\sigma t} \frac{\partial}{\partial t} c_{\sigma t} - U \tilde{n}_{\uparrow t} \tilde{n}_{\downarrow t} \right).$$

Here $\tilde{n}_{\sigma t} \equiv \frac{1}{2}(\bar{c}_{\sigma t-0} c_{\sigma t} + \bar{c}_{\sigma t+0} c_{\sigma t})$, so that there is a particle-hole symmetry of S_{at} (in a Hamiltonian notation, this would correspond to $U(n_\uparrow - \frac{1}{2})(n_\downarrow - \frac{1}{2})$ interaction term) [14].

We suppose an adiabatic switch of the hybridization as time goes to infinity. Formally this means that Δ is multiplied by a slow profile function $\Delta^{\text{prof}}(t)$ such as $\Delta^{\text{prof}}(\pm\infty) = 0$ and $\Delta^{\text{prof}}(t) = 1$ otherwise. In this case, the evolution starts and finishes with a bare atom having a single electron. The complete evolution operator $\mathcal{S}(-\infty, \infty)$ preserves the spin orientation. Therefore, it can be divided into the two parts, responsible for the evolution that starts and finishes with a certain spin orientation:

$$\mathcal{S} = \mathcal{S}_{\uparrow\uparrow} + \mathcal{S}_{\downarrow\downarrow}, \tag{1}$$

where $\mathcal{S}_{\uparrow\uparrow}$ and $\mathcal{S}_{\downarrow\downarrow}$ describe the evolution $|\uparrow\rangle_{-\infty} \to |\uparrow\rangle_{+\infty}$ and $|\downarrow\rangle_{-\infty} \to |\downarrow\rangle_{+\infty}$. Formally, $\mathcal{S}_{\sigma\sigma}$ can be defined as

$$\mathcal{S}_{\sigma\sigma} = \int_{|\sigma\rangle}^{|\sigma\rangle} e^{iS} \mathcal{D}[\bar{c}c], \tag{2}$$

where $\int_{|\sigma\rangle}^{|\sigma\rangle} \mathcal{D}[\bar{c}c]$ implies integration over the trajectories starting and finishing with a definite spin orientation. Such a trick is necessary due to degenerate ground state of the atomic Hamiltonian. For usual stationary diagrammatic technique, the ground state is unique, and therefore always evolves to itself at infinite time.

In practice, it is enough to consider only one part of the evolution operator, for example $\mathcal{S}_{\uparrow\uparrow}$. The account of another part is equivalent to spin-averaging of the results obtained.

Preliminary analysis. A transformation to the dual variables [13] requires a splitting of the action into two parts. The first part might be nonlinear but should be exactly solvable, and the second part is supposed to be Gaussian. The simplest way is to choose S_{at} and hybridization as those parts. Such a theory will be developed in the next sections. It will be shown that it describes the low-energy physics quite good. However, a correct description of all frequencies range requires a more sophisticated approach, and a renormalization procedure will be introduced.

A Hubbard-Stratonovich decoupling of the hybridization term and subsequent integration over $\bar{c}, c$ in the evolution operator results in the dual action

$$S[\bar{f}, f] = \sum_\sigma \int_{-\infty}^{+\infty} d\epsilon \left(\Delta_\epsilon^{-1} g_{\sigma\sigma,\epsilon}^{-2} - g_{\sigma\sigma,\epsilon}^{-1} \right) \bar{f}_{\sigma,\epsilon} f_{\sigma,\epsilon} + V[\bar{f}, f], \tag{3}$$

where $g_{\sigma\sigma,\epsilon}$ is an atomic Green's function, $g_{12} = -i\langle c_1 \bar{c}_2 \rangle$, and Taylor coefficients of the nonlinear part $V[\bar{f}, f]$ are vertexes of the atomic problem (see [13, 11] for detailed discussion).

Momenta of the atomic problem can be calculated in the time domain, using world-line representation. Parts (a) and (b) of the Fig.1 show nonvanishing world lines

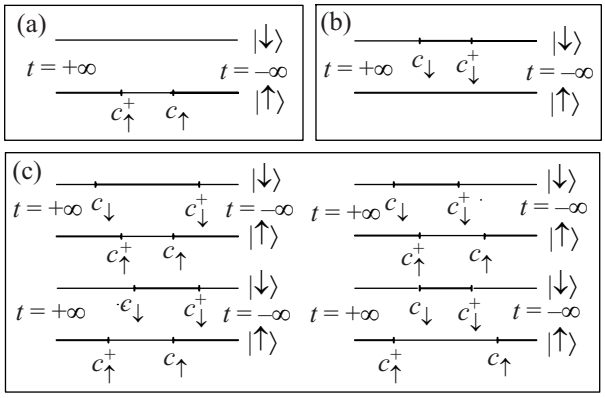

Fig.1. The world-lines contributing to $g_{\sigma\sigma}$ (a,b) and $\gamma^{(4)}_{\uparrow\downarrow\uparrow\downarrow}$ (c)

describing the calculation of the Green's function. One can see that there is a definite ordering of the creation-annihilation operators, since the evolution starts and finishes with a single electron with the spin-up orientation: annihilation should precede creation for spin-up and vice versa for spin-down operators. At the half-filling case one obtains $g_{\uparrow\uparrow}(t) = i\theta(-t)e^{i(U/2)t}$ and $g_{\downarrow\downarrow}(t) = -i\theta(t)e^{-i(U/2)t}$ (θ is a Heaviside step function). The Fourier transformation gives

$$g_{\uparrow\uparrow}(\epsilon) = \frac{1}{\epsilon + U/2 - i0}, \quad g_{\downarrow\downarrow}(\epsilon) = \frac{1}{\epsilon - U/2 + i0}. \tag{4}$$

These formulas are sufficient to construct the mean-field approximation, as higher momenta does not enter the theory in that case. In the line with the paper [13], one obtains

$$\mathcal{G}_{\sigma\sigma}(\epsilon) = \left(g_{\sigma\sigma}^{-1}(\epsilon) - \Delta(\epsilon) \right)^{-1},$$
$$\mathcal{G}_{\sigma\sigma}^{dual}(\epsilon) = \mathcal{G}_{\sigma\sigma}(\epsilon) - g_{\sigma\sigma}(\epsilon). \tag{5}$$

Through the paper the mean-field results are denoted with the calligraphic letters.

An average over spin indices should be taken to obtain the final result:

$$\mathcal{G}(\epsilon) = \frac{1/2}{\epsilon + U/2 - \Delta(\epsilon) - i0} + \frac{1/2}{\epsilon - U/2 - \Delta(\epsilon) + i0}. \tag{6}$$

In our notation, quantities before and after spin averaging are marked with the same letters. To prevent a confusion, we always supply the non-averaged quantities with spin indices.

We will be mostly interested in Kondo-like problem, so that atomic resonances $\pm U/2$ lie outside the conduction band. One can see the mean-field DOS of such a problem is built of slightly reshaped band DOS and two δ-peaks at $\pm U/2$. The main limitation of this approximation is that no Kondo peak appears near Fermi level, while the higher-energy part of DOS is qualitatively correct.

Low-energy properties: general consideration. A calculation of corrections to the mean-field theory requires knowledge of higher momenta of the atomic problem. The two-particle Green's function $g^{(2)}_{1234} = \langle c_1 c_2 c_3^\dagger c_4^\dagger \rangle$ can be calculated similarly to g_{12} (indices here are combinations of energy and spin, for instance 1 stands for ϵ_1, σ_1). The expression for $g^{(2)}$ contains 24 different terms, corresponding to various mutual order of the four time and spin arguments. However it turns out that only four of those terms contribute to the non-Gaussian part $\Gamma_{1234} = g^{(2)}_{1234} - g_{13}g_{24} + g_{14}g_{23}$. The world lines corresponding to these terms are depicted in part (c) of Fig.1. After the Fourier transform (omitting the energy-conserving delta function), we obtain a simple formula for the fourth-order vertex $\gamma^{(4)}_{1234} = -ig^{-1}_{11}g^{-1}_{22}g^{-1}_{33}g^{-1}_{44}\Gamma_{1234}$. The four-point vertex for all-the-same spin indices is equal to zero, and for the different indices has the following simple form:

$$\gamma^{(4)}_{\uparrow\downarrow\uparrow\downarrow}(\epsilon_1, \epsilon_2; \epsilon_3, \epsilon_4) = U + \frac{U^2}{\epsilon_3 - \epsilon_2 - 0i}. \tag{7}$$

The first term of this expression is local in time, whereas the second one is proportional to $\theta(t_3 - t_1)\delta(t_4 - t_1)\delta(t_3 - t_2)$ in time-domain. The Heaviside function appears here because of the degeneracy of the ground state: a time interval between the pairs t_1t_4 and t_2t_3 can be arbitrary large (see Fig.1).

The dual-fermion approach is essentially based on a diagrammatic expansion with respect to $\gamma^{(4)}$. Here it is worth to note that for the system without symmetry break [11] $\gamma^{(4)} \to \infty$ as temperature goes to zero, making such an expansion impossible. Therefore the symmetry breaking solution is indeed necessary to construct a zero-temperature theory.

We restrict ourselves with the simplest approximation beyond mean-field, that is a first-order diagram correction to the dual self-energy:

$$\Sigma^{dual}_{\uparrow\uparrow}(\epsilon) = \frac{i}{2\pi}\int \gamma^{(4)}_{\uparrow\downarrow\uparrow\downarrow}(\epsilon, \epsilon'; \epsilon, \epsilon')\mathcal{G}^{dual}_{\downarrow\downarrow}(\epsilon')d\epsilon' \tag{8}$$

and similarly for $\Sigma^{dual}_{\downarrow\downarrow}$. It would be more accurate to use the integrand with the dressed dual Green's function $G^{dual}_{\downarrow\downarrow}$, but we will stay with bare $\mathcal{G}^{dual}_{\downarrow\downarrow}$ for simplicity.

In order to obtain an expression for the Green's function, it is practical to use the following identity [13]:

$$G_{\sigma\sigma}(\epsilon) = \frac{1}{g^{-1}_{\sigma\sigma}(\epsilon) - \Delta(\epsilon) - \left(g_{\sigma\sigma}(\epsilon) + (\Sigma^{dual}_{\sigma\sigma}(\epsilon))^{-1}\right)^{-1}}. \tag{9}$$

An important property of these formulas is that $\Sigma^{dual}_{\sigma\sigma}$ contains the Kondo logarithm. Indeed, substituting (7) into (8) and taking into account that $\operatorname{Im}\mathcal{G}^{dual}$ changes its sign at the Fermi level, one finds that $\operatorname{Re}\Sigma^{dual}_{\uparrow\uparrow}$ contains the logarithmic singularity: $(2\pi)^{-1}\int \frac{U^2}{\epsilon - \epsilon' - i0}\operatorname{Im}\mathcal{G}^{dual}_{\downarrow\downarrow}(\epsilon')d\epsilon' \approx \pi^{-1}U^2\log(-\Omega/\epsilon)\operatorname{Im}\mathcal{G}^{dual}_{\downarrow\downarrow}(-0)$, where the cut-off Ω is about the half-bandwidth. Further the substitution of Eq. (5) gives an estimation $\operatorname{Re}\Sigma^{dual}_{\uparrow\uparrow} \approx 2\pi^{-1}\log(-\Omega/\epsilon)$ for the case of large U. Such a logarithmic behavior is also reflected in spectral function.

The dual perturbation theory is valid while the corrections to the mean-field result are small enough. According to formula (9), it means that the domain of validity is determined by the inequality $g_{\uparrow\uparrow}\Sigma_{\uparrow\uparrow} \ll 1$. Note that at the Kondo energy [15] $\epsilon_K \propto \exp(-\frac{\pi U}{8})$ the left-hand side of this inequality equals one-half, so our theory is formally valid only above the Kondo scale. But it is important to note that some of low-energy physics is also reproduced. Namely, Friedel sum rule [15] is satisfied: as one can see from (9), the divergence of $\Sigma^{dual}_{\sigma\sigma}$ corresponds to $G_{\sigma\sigma} = -\Delta^{-1}$.

It might be interesting to observe that the situation is similar for higher-order diagrams. The n-th order diagram for $\Sigma^{dual}_{\sigma\sigma}$ contains n nodes and $2n-1$ inner line. Above the Kondo scale, vertices are proportional to U^2 (see Eq. (7)) and each inner line $\mathcal{G}^{dual}_{\sigma\sigma}$ is proportional to U^{-2} for $U \to \infty$ (see Eq. (5)). Thereby the theory behaves well above Kondo scale.

Low-energy properties: analytical results for a semicircular bath. An explicit calculation of the first-order diagram in dual variables is a simple though not trivial task. The bare dual Green's function $\mathcal{G}^{dual}_{\uparrow\uparrow}(\epsilon)$ has an atomic pole at $-U/2$ (and at $U/2$ for $\mathcal{G}^{dual}_{\downarrow\downarrow}(\epsilon)$) as well as a branch cut originating from the fact that $\Delta(\epsilon)$ represents a system with a continuous spectrum.

In our calculation we will use a semicircular $\Delta(\epsilon)$:

$$\Delta(\epsilon) = \frac{1}{2}\left(\frac{2t}{D}\right)^2 (\epsilon - \mathrm{sgn}(\epsilon)\sqrt{\epsilon^2 - D^2}). \qquad (10)$$

Here D is the half-bandwidth, which for simplicity is put to one in all calculations below. Hybridization constant t describes the coupling between the impurity atom and its nearest neighbor. A calculation of the first-order diagram with a generic $\Delta(\epsilon)$ is obviously possible and requires only additional one-dimensional numerical integration. As it follows from the previous section, the result will be qualitatively similar for any $\Delta(\epsilon)$ which is smooth at $\epsilon = 0$ and has a finite bandwidth.

The diagram we are going to calculate is an integral over the real axis:

$$\Sigma^{dual}_{\uparrow\uparrow}(\epsilon) = -i\int \frac{d\epsilon'}{2\pi}\left(U + \frac{U^2}{\epsilon - \epsilon' - i0}\right)\mathcal{G}^{dual}_{\downarrow\downarrow}(\epsilon'), \quad (11)$$

$$\Sigma^{dual}_{\downarrow\downarrow}(\epsilon) = -i\int \frac{d\epsilon'}{2\pi}\left(U + \frac{U^2}{\epsilon' - \epsilon - i0}\right)\mathcal{G}^{dual}_{\uparrow\uparrow}(\epsilon'). \quad (12)$$

Let us examine the pole structure of the part proportional to U (a constant part) in the expression for $\Sigma^{dual}_{\uparrow\uparrow}(\epsilon)$. Denote this part Σ^{dual}_U,

$$\Sigma^{dual}_U = -i\frac{U}{2\pi}\int \frac{\Delta(\epsilon')\, d\epsilon'}{(\epsilon' - U/2 + i0)(\epsilon' - U/2 + i0 - \Delta(\epsilon'))}. \qquad (13)$$

There is a pole at $\epsilon' = U/2 - i0$ inherited from the atomic problem, in addition there are at most two poles which are solutions of the equation $\epsilon - U/2 = \Delta(\epsilon)$. For our special choice of $\Delta(\epsilon)$ this equation is reducible to the following system:

$$\begin{cases} \mathrm{Re}\,\Delta(\epsilon) &= \epsilon - U/2 \\ \mathrm{Im}\,\Delta(\epsilon) &= 0 \end{cases} \Leftrightarrow$$

$$\begin{cases} \epsilon^2(1-4t^2) + \epsilon U(2t^2-1) + ((2t^2)^2 + (U/2)^2) = 0 \\ |\epsilon| > 1 \end{cases}. \qquad (14)$$

In the case of $t = 1/2$ this quadratic equation turns to a linear one and its root $\epsilon_0 = \frac{1}{2}\left(U + \frac{1}{U}\right)$ is always greater than or equal to 1. When t is not equal to $1/2$, two real roots ϵ_+ and ϵ_- are possible. This is a manifestation of an additional state of the discrete spectrum due to the impurity. However in the limit $U \gg 2t$ the only relevant root is still ϵ_+. To understand this statement it's useful to represent $\mathrm{Re}\,\Delta(\epsilon) = \epsilon - U/2$ equation in a graphical form (see the Fig.2).

As one can see, the magnitude of t determines the height of "shoulders" in this figure, while $U/2$ is a vertical displacement of the diagonal line $\epsilon - U/2$. At U large

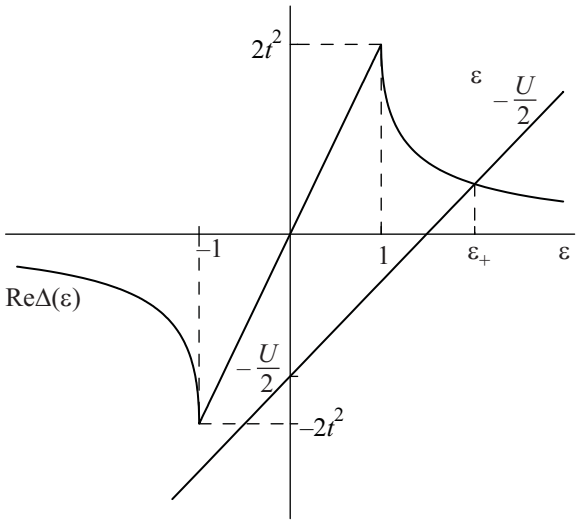

Fig.2. Graphical solution of the equation $\mathrm{Re}\,\Delta(\epsilon) = \epsilon - U/2$

enough in comparison with $2t^2$ (dimensionless) there is only one intersection of the curves on the positive half-axis, i.e. ϵ_+. A complete analysis of this equation yields the following results:

t, U	Roots
$t = 1/2$	$\epsilon = \frac{1}{2}\left(U + \frac{1}{U}\right)$
$t \neq 1/2,\ 2t^2 < 1, U/2 < 1 - 2t^2$	no real roots
$t \neq 1/2, U/2 > \lvert 1 - 2t^2\rvert$	$\epsilon = \epsilon_+$
$2t^2 \geq 1,\ U/2 \leq 2t^2 - 1$	$\epsilon = \epsilon_+, \epsilon_-$

$$\epsilon_\pm = \frac{(U/2)(4t^2-2) \pm 4t^2\sqrt{4t^2 + (U/2)^2 - 1}}{2(4t^2-1)}. \qquad (15)$$

The both poles $U/2 - i0$ and $\epsilon_+ - i0$ reside in the fourth quadrant while $\Delta(\epsilon)$ has a branch cut on $[-1;1]$. To preserve causality it has to perform an infinitesimal shift up where $\epsilon < 0$ and down for $\epsilon > 0$. Such a disposition of the poles permits us to choose an integration contour in the upper half-plane (the integrand vanishes at infinity as ϵ^{-3}) and then deform it to a smaller contour C as shown in Fig.3.

Further, the integrand of Σ^{dual}_U can be split into two parts as follows

$$\Sigma^{dual}_U = -i\frac{U}{2\pi}\times$$

$$\times \oint_C d\epsilon' \left(\frac{1}{\epsilon' - U/2 + i0 - \Delta(\epsilon')} - \frac{1}{\epsilon' - U/2 + i0}\right).$$

One can observe that the second term of the integrand does not contribute to the result, since it contains no singularities in the contour. To proceed with the first

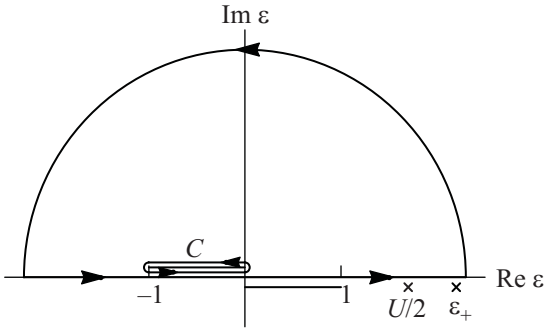

Fig.3. Contour of integration for the constant part of $\Sigma^{dual}_{\uparrow\uparrow}(\epsilon)$

term, we substitute the explicit expressions for real and imaginary parts of Δ and take into account that imaginary part changes its sign under a transition from one side of the branch cut to another. After some transformations we obtain

$$\Sigma^{dual}_U = \frac{U}{2\pi}\frac{4t^2}{1-4t^2}\int_{-1}^{0}\frac{\sqrt{1-\epsilon'^2}d\epsilon'}{(\epsilon'-\epsilon_+)(\epsilon'-\epsilon_-)}. \quad (16)$$

This integral can be simply evaluated by a trigonometric substitution $\epsilon' = \sin\phi$. Finally, we obtain the following result:

$$\Sigma^{dual}_U = \frac{U}{2\pi}\frac{4t^2}{1-4t^2}\left(-\frac{\pi}{2}+\frac{L(\epsilon_+)-L(\epsilon_-)}{\epsilon_+-\epsilon_-}\right), \quad (17)$$

$$L(x) \equiv \sqrt{1-x^2}\log\left(\frac{\sqrt{1-x^2}+x-1}{\sqrt{1-x^2}-x+1}\right). \quad (18)$$

There is no need to repeat all calculations for the second part of vertex (proportional to U^2) (11). An additional multiplier $(\epsilon-\epsilon'-i0)^{-1}$ produces another pole below the real axis, so it doesn't affect the integration contour in any way. This means that the last integral in (16) should be replaced with

$$\int_{-1}^{0}\frac{d\epsilon'\sqrt{1-\epsilon'^2}}{(\epsilon-\epsilon'-i0)(\epsilon'-\epsilon_+)(\epsilon'-\epsilon_-)} = \\ = \frac{1}{\epsilon_+-\epsilon_-}\int_{-1}^{0}\frac{d\epsilon'\sqrt{1-\epsilon'^2}}{\epsilon-\epsilon'-i0}\left(\frac{1}{\epsilon'-\epsilon_+}-\frac{1}{\epsilon'-\epsilon_-}\right).$$

In this way we have reduced the U^2-part to a known result. The final expression for $\Sigma^{dual}_{\uparrow\uparrow}(\epsilon)$ reads:

$$\Sigma^{dual}_{\uparrow\uparrow}(\epsilon) = \frac{U}{2\pi}\frac{4t^2}{1-4t^2}\left(-\frac{\pi}{2}+\frac{L(\epsilon_-)-L(\epsilon_+)}{\epsilon_--\epsilon_+}+ \right. \\ \left. \frac{U}{\epsilon_+-\epsilon_-}\left(\frac{L(\epsilon-i0)-L(\epsilon_-)}{\epsilon-\epsilon_-}-\frac{L(\epsilon-i0)-L(\epsilon_+)}{\epsilon-\epsilon_+}\right)\right). \quad (19)$$

An infinitesimal imaginary part in $L(\epsilon-i0)$ assists to choose the right side of the branch cut. Such an imaginary addition is not required for $\epsilon_\pm$, since they do not lie on the brunch cut for any positive t and U.

An evaluation of $\Sigma^{dual}_{\downarrow\downarrow}(\epsilon)$ repeats the previous one with a number of exceptions:

- Poles of the integrand are at $-U/2+i0$ and $-\epsilon_+ + i0$.
- The integration contour goes in the opposite direction and surrounds $[0;1]$ segment.
- The pole of $(\epsilon'-\epsilon-i0)^{-1}$ lies above the real axis.

So we have a very similar answer:

$$\Sigma^{dual}_{\downarrow\downarrow}(\epsilon) = -\Sigma^{dual}_{\uparrow\uparrow}(-\epsilon). \quad (20)$$

By taking a limit of $t \to 1/2$ in formula (19) we achieve even simpler expression:

$$\Sigma^{dual}_{\uparrow\uparrow}(\epsilon)|_{t=1/2} = -\Sigma^{dual}_{\downarrow\downarrow}(-\epsilon)|_{t=1/2} = \\ = \frac{\epsilon_0-U}{2}-\frac{1}{\pi}\left(1+L(\epsilon_0)-U\frac{L(\epsilon_0)-L(\epsilon-i0)}{\epsilon_0-\epsilon}\right), \\ \epsilon_0 = \frac{1}{2}(U+1/U). \quad (21)$$

This result for dual self energy should be put into the formula for Green's function (9). We have plotted thus obtained DOS for several values of U and obtained smooth graphs with a clear Kondo-like peak at the Fermi level.

We found however, that the simplest first-order theory suffers serious problems at higher frequencies. This issue is discussed in the next section.

Renormalization procedure. The mentioned drawbacks of the formalism presented so far are related to the poles of $g_{\sigma\sigma}(\epsilon)$. First of all, as it follows from Eq. (9), the Green's function $G_{\sigma\sigma}$ is pinned at its mean-field value $-1/\Delta$ at these energy points. The only case when this pinning is absent is the vanishing of $\Sigma^{dual}_{\sigma\sigma}$ at the energy of the pole, but it seems that no finite-order approximation for $G_{\sigma\sigma}(\epsilon)$ provides such a condition. The pinning is rather unphysical, because poles of the atomic problem are by no means special points for the entire action (1), and there is no any sum rule about them. Further analysis shows that the theory fails also near the poles of the atomic problem: it replaces the mean-field pole $\epsilon = U/2 - \Delta(\epsilon)$ with the two poles shifted from the real axis in different directions. Consequently, the theory is neither conservative, nor causal.

The problems with the poles of $g_{\sigma\sigma}(\epsilon)$ are probably related to the pole structure of the dual Green's function.

As it follows from the second line of Eq.(5), it has two close poles, one of them is placed exactly at $U/2$ while another is slightly shifted from this point. The residues of these poles have the opposite signs. We suppose that the series expansion breaks down in this region. We propose the following renormalization procedure. Since the pinning is absent only if dual self-energy vanishes at the pole,

$$G_{\sigma\sigma}(\epsilon_{\text{pole}}) = 0; \quad g^{-1}_{\sigma\sigma}(\epsilon_{\text{pole}}) = 0, \tag{22}$$

its reasonable to *require* the fulfillment of this condition. An additional condition means that the theory must have a renormalization parameter. To introduce it, we modify the splitting of the action into the Gaussian and Hamiltonian parts. We rewrite the action (1) as follows:

$$S = S'_{at} - \iint_{-\infty}^{+\infty} dt dt' \bar{c}_{\sigma t} \left(\Delta(t-t') + i\lambda\delta'(t-t')\right) c_{\sigma t'},$$
$$S'_{at} = \int_{-\infty}^{+\infty} dt \left(i(1-\lambda)\bar{c}_{\sigma t}\frac{\partial}{\partial t} c_{\sigma t} - U\tilde{n}_{\uparrow t}\tilde{n}_{\downarrow t} + \mu\tilde{n}_{\sigma t}\right). \tag{23}$$

The parameter λ is to be adjusted to maintain the condition (22). One can observe similiarities with the field-theory renormalization procedure, that is a way to solve divergence problems by redefinition of physical constants, for example, masses and interaction constants.

The calculations are very similar to the above considered case $\lambda = 0$. The atomic problem is the same, up to scaling transformations. We obtain the following relations:

$$g_{\sigma\sigma}(\epsilon) = \left((1-\lambda)\epsilon \pm U'/2 \mp i0\right)^{-1}; \; U' \equiv (1-\lambda)^{-1}U,$$
$$\gamma^{(4)}_{\uparrow\downarrow\uparrow\downarrow}(\epsilon_1, \epsilon_2; \epsilon_3, \epsilon_4) = U + \frac{U'^2}{\epsilon_3 - \epsilon_2 - 0i}. \tag{24}$$

The mean-field approximation gives

$$\mathcal{G}_{\sigma\sigma}(\epsilon) = \left(\epsilon \pm U' - \Delta(\epsilon) \mp i0\right)^{-1}, \tag{25}$$

so that the renormalization is just results in a shift of the atomic resonances. Practical calculation shows that (22) is fulfilled with a small positive λ, and that λ grows as U decreases.

A calculation of the first-order correction within the renormalization scheme is also similar. The only important difference is that $\mathcal{G}^{dual}_{\sigma\sigma}(\epsilon)$ obeys high frequency asymptotic $\frac{\lambda}{1-\lambda}\epsilon^{-1}$ for a finite λ, and therefore the contour integration contains an additional contribution from infinity. The final formula for the dual self-energy(19) becomes:

$$\Sigma^{dual}_{\uparrow\uparrow}(\epsilon;\lambda) = -\Sigma^{dual}_{\downarrow\downarrow}(-\epsilon;\lambda) =$$
$$= \frac{U}{2\pi}\frac{4t^2}{1-4t^2}\left(-\frac{\pi}{2} + \frac{L(\epsilon'_-) - L(\epsilon'_+)}{\epsilon'_- - \epsilon'_+}\right) +$$
$$\frac{U'^2}{2\pi}\frac{4t^2}{1-4t^2}\frac{1}{\epsilon'_+ - \epsilon'_-}\left(\frac{L(\epsilon - i0) - L(\epsilon'_-)}{\epsilon - \epsilon'_-} - \right.$$
$$\left. \frac{L(\epsilon - i0) - L(\epsilon'_+)}{\epsilon - \epsilon'_+}\right) + \lambda\frac{U'}{2}$$
$$\epsilon'_\pm = \frac{(U'/2)(4t^2-2) \pm 4t^2\sqrt{4t^2 + (U'/2)^2 - 1}}{2(4t^2-1)} \tag{26}$$

Besides the renormalized band DOS, there are also separated poles, corresponding to the atomic resonances. Their positions are shown in the Fig.4. For comparison, we also plot the mean-field values with and without renormalization (poles of the expressions (25) and (5), respectively). It can be verified, that the renormalized theory is causal (that is, poles are infinitesimally shifted from the real axis in proper quadrants) and conservative (that is, the Luttinger theorem is fulfilled).

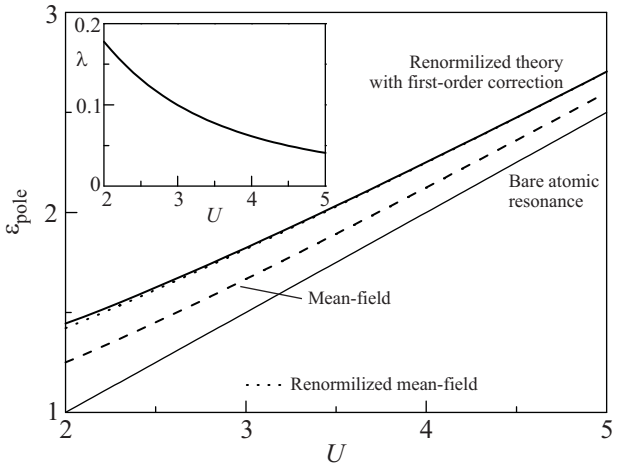

Fig.4. Position of the atomic resonance of SIAM with $t = D/2$ in different approximations. The resonance bare atom (that is, $\epsilon_{pole} = \frac{U}{2}$) is shown for comparison. Note that the renormalized theory gives a twice-larger shift of the resonance position than the mean-field approach does. For the renormalized theory, Σ vanishes near the resonance point, therefore taking the dual correction into account almost does not affect the resonance. Inset shows the value of renormalization parameter λ

We have performed calculations with this dual self-energy substituted in Eq. (9). The value of λ has been adjusted numerically to fulfill the condition (22). The resulting graphs for the impurity DOS are shown in Fig.5.

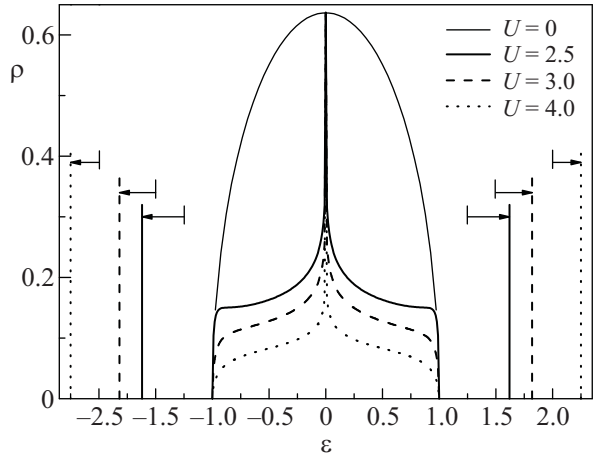

Fig.5. Local density of states $\rho(\epsilon) = -[\mathrm{sgn}(\epsilon)/\pi]\,\mathrm{Im}\,G(\epsilon)$ of SIAM with $t = D/2$, calculated from the renormalized theory. Atomic resonances are shown with vertical lines; height of the line is determined by the spectral weight of the resonance. Arrows indicate shift from the resonance of the bare atom

Conclusion. To conclude, the presented first-order analytical scheme catches the physics of the SIAM at different energy scales, including the Kondo-like peak near Fermi level and a shift of isolated atomic resonances due to hybridization with the conduction band. Our construction of the expansion around atomic problem with a degenerate ground state required us to introduce the symmetry break and renormalization procedures, that are vital parts of the presented theory.

Finally, we can compare our scheme to the approach by Logan et al [10], since the local moment approach developed there is formally equivalent to the present theory in a number of points. A similar form of the bare Green's functions is used to construct a diagrammatic expansion. Nevertheless, the Green's functions of the local moment approach are to be determined self-consistently, so that it includes poles of a partially "dressed" impurity atom. In the same fashion summation of ladder diagrams is required to obtain a renormalized energy-dependent vertex having a necessary anomaly near zero frequency. So, the approach proposed by D. Logan requires an essential numerics. In contrast, we presented an almost analytical scheme. Therefore, the result can be improved in a regular way by the account of higher-order diagrams. Another important feature of our approach is related with the renormalization procedure of atomic levels due to hybridization with conduction electrons. A crucial checkpoint for the further development of the present method is related with applicability to multi-orbital systems. As far as we know, the Logan's approach has met serious difficulties beyond single-band systems, although there is a promising result of the variational scheme [16]. For the present scheme multi-orbital generalization looks straightforward.

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