The Kondo effect in periodic narrow-band systems

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Abstract. The Kondo divergences owing to interaction of current carriers with local moments in highly correlated electron systems are considered within the Hubbard and s-d exchange models with infinitely strong on-site interaction, the many-electron Hubbard representation being used. The picture of density of states containing a peak at the Fermi level is obtained. Various forms of the self-consistent approximation are used. The problem of the violation of analytical properties of the Green's function is discussed. Smearing of the "Kondo" peak owing to spin dynamics and finite temperatures is investigated.

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The problem of strong correlations and magnetism in many-electron systems is one of the most important in the solid state theory. Since the Hubbard's works of 60's, a great progress has been achieved in understanding electronic structure of systems with strong on-site interaction. Last time, the role of the Kondo effect has been discussed within the large-d approach (d is space dimensionality) which reduces the initial periodic Hubbard model to an effective Anderson impurity model [1,2]. Besides the Hubbard bands, an important role in the formation of density of states (DOS) picture belongs to a peak at the Fermi level, which was found for both half-filled and doped case (the latter case is considered in [2,3]). It should be noted that this approach meets with a number of computational difficulties (*e.g.*, consideration of finite temperatures is needed, and the low-temperature limit is non-trivial). The structure of the spectrum in large-d approaches is confirmed by the Monte-Carlo calculations. On the other hand, this feature was not reproduced by most preceding analytical approaches. In particular, the Hubbard-III approximation [4] does not take into account contributions of Fermi-like excitations in a proper way because of its single-site character. A detailed analysis of this approximation was performed in references [5,6] within the large-z (z is nearest-neighbor number) expansion.

In the present paper we present a treatment that is based on the method of equations of motion for the many-electron Hubbard operators [7,8] and is much more simple than the large-d approach. As the zero order this approach reduces to the simplest Hubbard-I approximation. General expressions for $1/z$-corrections were obtained in reference [5]. Unfortunately, the terms with the one-particle occupation numbers (which just describe the

Kondo effect) were neglected in references [5,6], and only a classical approximation was considered in reference [6].

We start from the s-d exchange model with the large s-d coupling parameter $|I|$,

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} t_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - I \sum_{i\sigma\sigma'} \mathbf{S}_i \boldsymbol{\sigma}_{\sigma\sigma'} c^{\dagger}_{i\sigma} c_{i\sigma'} + \mathcal{H}_d, \qquad (1)$$

where $t_{\mathbf{k}}$ is the band energy, $\mathcal{H}_d$ is the Heisenberg Hamiltonian of the localized-spin system, $\boldsymbol{\sigma}$ are the Pauli matrices. In the limit $|I| \to \alpha\infty$ (here and hereafter $\alpha = \text{sign } I = \pm$), it is convenient to pass to the atomic representation of the Hubbard operators $X_i^{\beta\gamma} = |i\beta\rangle\langle i\gamma|$ where $\mathcal{H}_{sd}$ (the second term in (1)) takes the diagonal form [9]. For the electron concentration $n < 1$, after performing the procedure of projection onto the corresponding state space, the one-electron Fermi operators $c^{\dagger}_{i\sigma}$ are replaced by the many-electron operators $g^{\dagger}_{i\sigma\alpha}$. These are expressed in terms of the X-operators as

$$g^{\dagger}_{i\sigma+} = \sum_M \{(S + \sigma M + 1)/(2S+1)\}^{1/2} X_i(M + \frac{\sigma}{2}, +; M),$$

$$g^{\dagger}_{i\sigma-} = \sum_M \sigma\{(S - \sigma M)/(2S+1)\}^{1/2} X_i(M + \frac{\sigma}{2}, -; M),$$

where $|M\rangle$ are the empty states and $|m\alpha\rangle$ are the singly-occupied states with the total on-site spin $S + \alpha/2$ and its projection m (which survive at $|I| \to \alpha\infty$), $\sigma = \pm$. The Hamiltonian of the s-d exchange interaction yields a constant energy shift only and can be omitted, so that we obtain

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} t_{\mathbf{k}} g^{\dagger}_{\mathbf{k}\sigma\alpha} g_{\mathbf{k}\sigma\alpha} + \mathcal{H}_d, \qquad \alpha = \text{sign } I. \qquad (2)$$

For $n > 1$ we have to pass to the "hole" representation by introducing new localized spins $\widetilde{S} = S \pm 1/2$, and

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the Hamiltonian takes the same form (2) with the replacement $t_{\mathbf{k}} \to -t_{\mathbf{k}}(2\widetilde{S}+1)/(2S+1)$. For $S = 1/2$, $I \to -\infty$ the Hamiltonian (2) coincides with that of the Hubbard model in the case of the infinite on-site repulsion $U \to \infty$ with the replacement $t_{\mathbf{k}} \to t_{\mathbf{k}}/2$ and the almost half-filled band, so that $n \to \delta$ with δ the hole concentration. Thus we do not need to discuss the Hubbard model separately (physically, both models describe the local-moment situation).

We calculate the one-particle Green's function for ferromagnetic (FM) state in the energy representation,

$$G_{\mathbf{k}\sigma\alpha}(E) = \langle\langle g_{\mathbf{k}\sigma\alpha}|g_{\mathbf{k}\sigma\alpha}^{\dagger}\rangle\rangle_E. \tag{3}$$

Using the commutation relations for the operators $g_{i\sigma\alpha}$ and spin operators (cf. Refs. [5,6]) we obtain the equation of motion

$$(E - t_{\mathbf{k}-\mathbf{q}\sigma\alpha})G_{\mathbf{k}\sigma\alpha}(E) = P_{\sigma\alpha}$$
$$+ \frac{\alpha}{2S+1}\sum_{\mathbf{q}} t_{\mathbf{k}-\mathbf{q}}\{\langle\langle\delta[\sigma S_{\text{tot}\mathbf{q}}^z$$
$$- \frac{1}{2}\sum_M X_{\mathbf{q}}(M\alpha; M\alpha)]g_{\mathbf{k}-\mathbf{q}\sigma\alpha}|g_{\mathbf{k}\sigma\alpha}^{\dagger}\rangle\rangle_E$$
$$+ \langle\langle S_{\text{tot}\mathbf{q}}^{-\sigma} g_{\mathbf{k}-\mathbf{q},-\sigma\alpha}|g_{\mathbf{k}\sigma\alpha}^{\dagger}\rangle\rangle_E\}, \tag{4}$$

with $S_{\text{tot}}^{\pm}$, S_{tot}^z being the total spin operators (including the contributions of empty and singly-occupied states, see for details [6]),

$$t_{\mathbf{k}\sigma\alpha} = P_{\sigma\alpha}t_{\mathbf{k}}, \qquad P_{\sigma\alpha} = \frac{\widetilde{S} + 1/2 + \alpha\sigma\langle S_{\text{tot}}^z\rangle - \alpha n/2}{2S+1},$$

$\langle S_{\text{tot}}^z\rangle$ is the total on-site average magnetization. The "Kondo" term comes from the last Green's function in the right-hand side of (4), which describes spin-flip processes. Performing decoupling of the next equation of motion to first order in the nearest-neighbor number $1/z$ we derive

$$(E - t_{\mathbf{k}-\mathbf{q}\sigma\alpha})\langle\langle S_{\text{tot}\mathbf{q}}^{-\sigma} g_{\mathbf{k}-\mathbf{q},-\sigma\alpha}|g_{\mathbf{k}\sigma\alpha}^{\dagger}\rangle\rangle_E =$$
$$\frac{\alpha}{2S+1}[\chi_{\mathbf{q}\sigma} + (2S+1)n_{\mathbf{k}-\mathbf{q}-\sigma\alpha}](1 + t_{\mathbf{k}}G_{\mathbf{k}\sigma\alpha}(E))$$
$$- \alpha n_{\mathbf{k}-\mathbf{q}-\sigma\alpha}t_{\mathbf{k}-\mathbf{q}}G_{\mathbf{k}\sigma\alpha}(E). \tag{5}$$

Here we have neglected $\mathcal{H}_d$,

$$\chi_{\mathbf{q}\sigma} = \langle S_{\text{tot}-\mathbf{q}}^{\sigma} S_{\text{tot}\mathbf{q}}^{-\sigma}\rangle, \qquad n_{\mathbf{k}\sigma\alpha} = \langle g_{\mathbf{k}\sigma\alpha}^{\dagger} g_{\mathbf{k}\sigma\alpha}\rangle.$$

To lowest order (i.e. in the Hubbard-I approximation) we have

$$n_{\mathbf{k}\sigma\alpha} = P_{\sigma\alpha}f(t_{\mathbf{k}\sigma\alpha})$$

where $f(E)$ is the Fermi function. After substituting (5) and a similar equation for the longitudinal contribution (which contains $\chi_{\mathbf{q}}^{zz} = \langle S_{\text{tot}-\mathbf{q}}^z S_{\text{tot}\mathbf{q}}^z\rangle$) into (4) we obtain

$$G_{\mathbf{k}\sigma\alpha}(E) = \frac{a_{\mathbf{k}\sigma\alpha}(E)}{b_{\mathbf{k}\sigma\alpha}(E) - a_{\mathbf{k}\sigma\alpha}(E)t_{\mathbf{k}}}, \tag{6}$$

where

$$a_{\mathbf{k}\sigma\alpha}(E) = P_{\sigma\alpha} + \sum_{\mathbf{q}} \frac{t_{\mathbf{k}-\mathbf{q}}}{(2S+1)^2}$$
$$\times \left[\frac{\chi_{\mathbf{q}\sigma} + (2S+1)n_{\mathbf{k}-\mathbf{q}-\sigma\alpha}}{E - t_{\mathbf{k}-\mathbf{q}-\sigma\alpha}} + \frac{\chi_{\mathbf{q}}^{zz}}{E - t_{\mathbf{k}-\mathbf{q}\sigma\alpha}}\right], \tag{7}$$
$$b_{\mathbf{k}\sigma\alpha}(E) = E - \sum_{\mathbf{q}} \frac{t_{\mathbf{k}-\mathbf{q}}^2}{2S+1}\frac{n_{\mathbf{k}-\mathbf{q}-\sigma\alpha}}{E - t_{\mathbf{k}-\mathbf{q}-\sigma\alpha}}. \tag{8}$$

The longitudinal fluctuations can be neglected in the saturated FM region [10], but are important in the paramagnetic region (the corresponding results are obtained from the above formulas at $\langle S_{\text{tot}}^z\rangle = 0$) which is considered hereafter. The equation for the chemical potential reads

$$\sum_{\mathbf{k}} \langle g_{\mathbf{k}\sigma\alpha}^{\dagger} g_{\mathbf{k}\sigma\alpha}\rangle = \frac{n}{2}.$$

To smear the logarithmic DOS singularity at the Fermi level, one has to take into account spin dynamics which is determined by the Hamiltonian $\mathcal{H}_d$ (cf. [11]). To this end, we introduce the normalized spectral spin function

$$K_{\mathbf{q}}(\omega) = -\frac{1}{\pi}N_{\text{B}}(\omega)\frac{\text{Im}\langle\langle S_{\mathbf{q}}^z|S_{-\mathbf{q}}^z\rangle\rangle_\omega}{\langle S_{-\mathbf{q}}^z S_{\mathbf{q}}^z\rangle}$$

where $N_{\text{B}}(\omega)$ is the Bose function. In the far paramagnetic region (where spin correlations can be neglected) we can use the simplest spin-diffusion approximation with

$$K_{\mathbf{q}}(\omega) = \frac{1}{\pi}\frac{Dq^2}{\omega^2 + (Dq^2)^2} \tag{9}$$

where D is the spin diffusion constant (in fact, the results depend weakly on the concrete form of spin dynamics). Then we have to put in (6)

$$a_{\mathbf{k}\alpha}(E) = P_\alpha + \sum_{\mathbf{q}} \int d\omega K_{\mathbf{q}}(\omega)\frac{t_{\mathbf{k}-\mathbf{q}}}{(2S+1)^2}$$
$$\times \frac{\chi + (2S+1)n_{\mathbf{k}-\mathbf{q}\alpha}}{E - P_\alpha t_{\mathbf{k}-\mathbf{q}} - \omega}, \tag{10}$$
$$b_{\mathbf{k}\alpha}(E) = E - \sum_{\mathbf{q}} \int d\omega K_{\mathbf{q}}(\omega)\frac{t_{\mathbf{k}-\mathbf{q}}^2}{2S+1}$$
$$\times \frac{n_{\mathbf{k}-\mathbf{q}\alpha}}{E - P_\alpha t_{\mathbf{k}-\mathbf{q}} - \omega}. \tag{11}$$

To simplify numerical calculations, we average the spectral function (9) in $\mathbf{q}$,

$$K_{\mathbf{q}}(\omega) \to \overline{K}(\omega) = \sum_{\mathbf{q}} K_{\mathbf{q}}(\omega),$$

which is sufficient to obtain qualitatively valid results. Indeed, this approximation (which is in spirit of the large-d or large-z expansion) reproduces correctly the low-frequency behavior of spin fluctuations which is important near the Fermi level. Then $a(E)$ and $b(E)$ do not depend
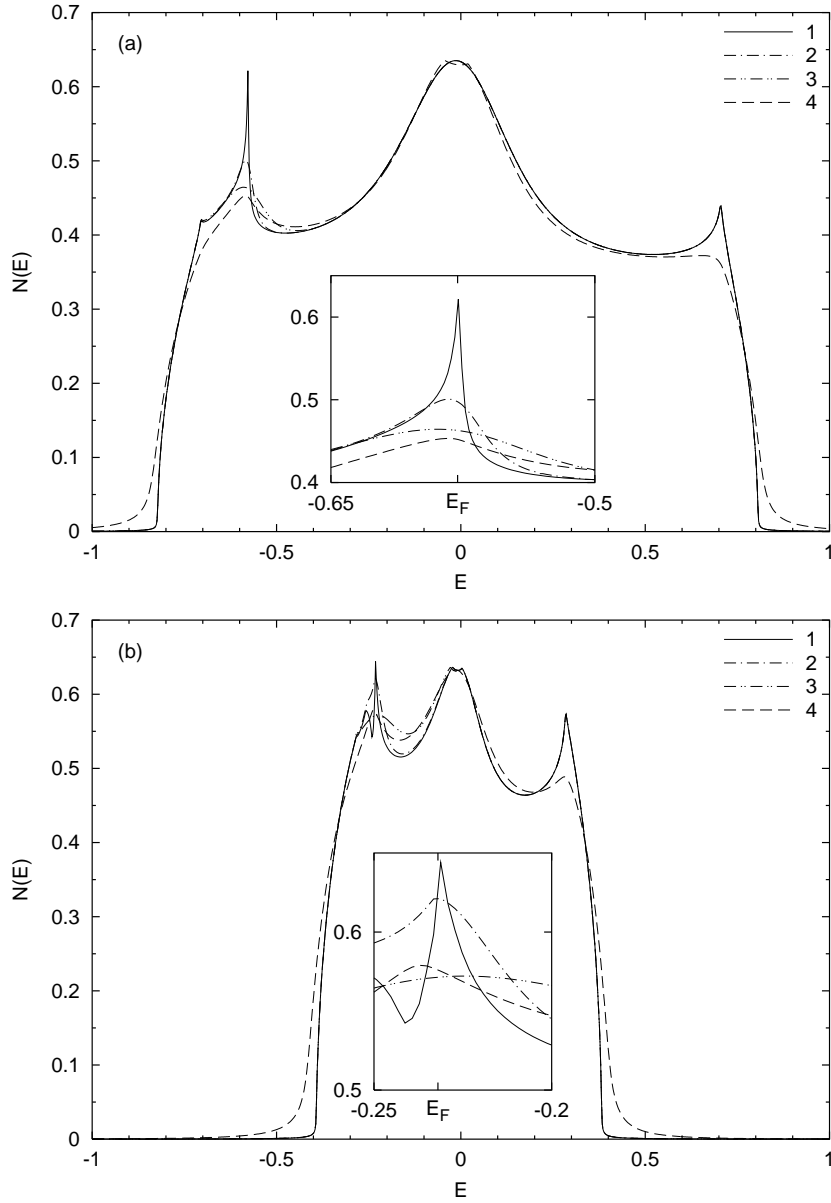
Fig. 1. The density of states picture for the Green's function (6) and semielliptic bare DOS with $S = 1/2$, $n = 0.15$ in the absence of spin dynamics for different temperatures (Eqs. (7, 8), lines 1, 2, 3 correspond to $T = 0, 0.01, 0.03$) and with account of spin dynamics at zero temperature (Eqs. (10, 11), line 4); (a) $\alpha = +$ and (b) $\alpha = -$. Inset shows the region near the Fermi energy which corresponds to the peak top. Energy and temperature is measured in units of bare half-bandwidth.

on **k**. We have taken below $D = 0.7c|t|$ (t is the transfer integral). In the far paramagnetic region we have

$$\langle (S_{\text{tot}}^z)^2 \rangle = \frac{1}{3}\langle \mathbf{S}_{\text{tot}}^2 \rangle = \frac{1}{3}\chi = \frac{1-n}{2S+1}\left(\frac{2}{3}S^3 + S^2 + \frac{1}{3}S\right)$$
$$+ \frac{n}{2\widetilde{S}+1}\left(\frac{2}{3}\widetilde{S}^3 + \widetilde{S}^2 + \frac{1}{3}\widetilde{S}\right).$$

Then we obtain for $S = 1/2$

$$\chi = \begin{cases} 3(1-n)/4 + 2n, & \alpha = +, \\ 3(1-n)/4, & \alpha = -. \end{cases}$$

The results of numerical calculation of the single-particle density of states

$$N_\alpha(E) = -\frac{1}{\pi}\operatorname{Im}\sum_{\mathbf{k}} G_{\mathbf{k}\alpha}(E) \qquad (12)$$

for the semielliptic bare DOS are shown in Figure 1. One can see that pronounced density of states peaks occur at the Fermi level. The peaks are smeared by both including spin dynamics and finite temperatures. It should be noted that, unlike the large-d approach [2], the limit of zero temperature makes no difficulties.
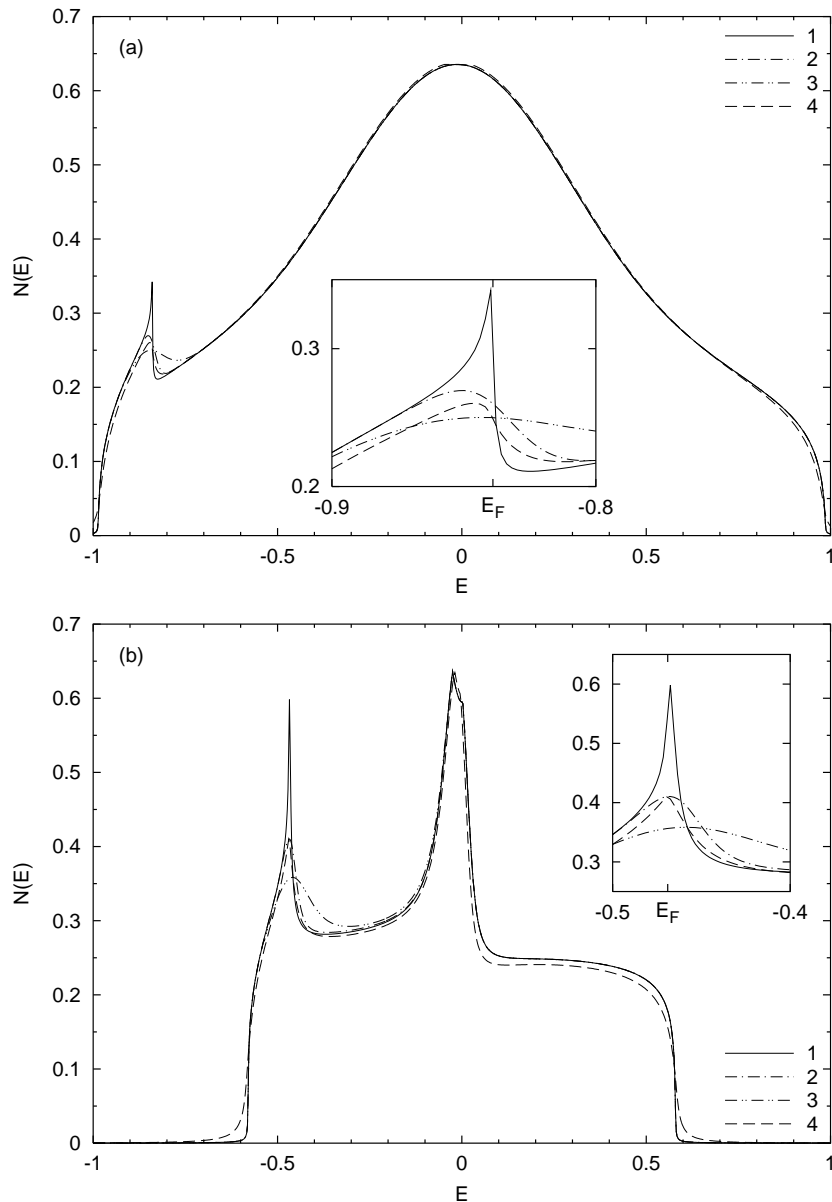
Fig. 2. The density of states picture in the self-consistent approximation (14) with $S = 1/2$, $n = 0.05$. The notations are the same as in Figure 1.

As well as for small-I Kondo problem, the "Kondo effect" is connected with the Fermi functions (which were not treated in Ref. [5]) and is a quantum effect that is small in $1/S$. Unlike the FM case, where the singularity has one-sided form and non-quasiparticle (incoherent) contributions to the density of state plays main role [10], the logarithmic contribution is symmetric with respect to the Fermi level. Note that after formal expansion in $1/z$ the contributions to the Green's function with the Fermi functions are canceled in the paramagnetic phase to first order [12].

As discussed in reference [5], the approximation (7, 8) leads to some formal difficulties connected with occurrence of an additional singularity of the Green's function
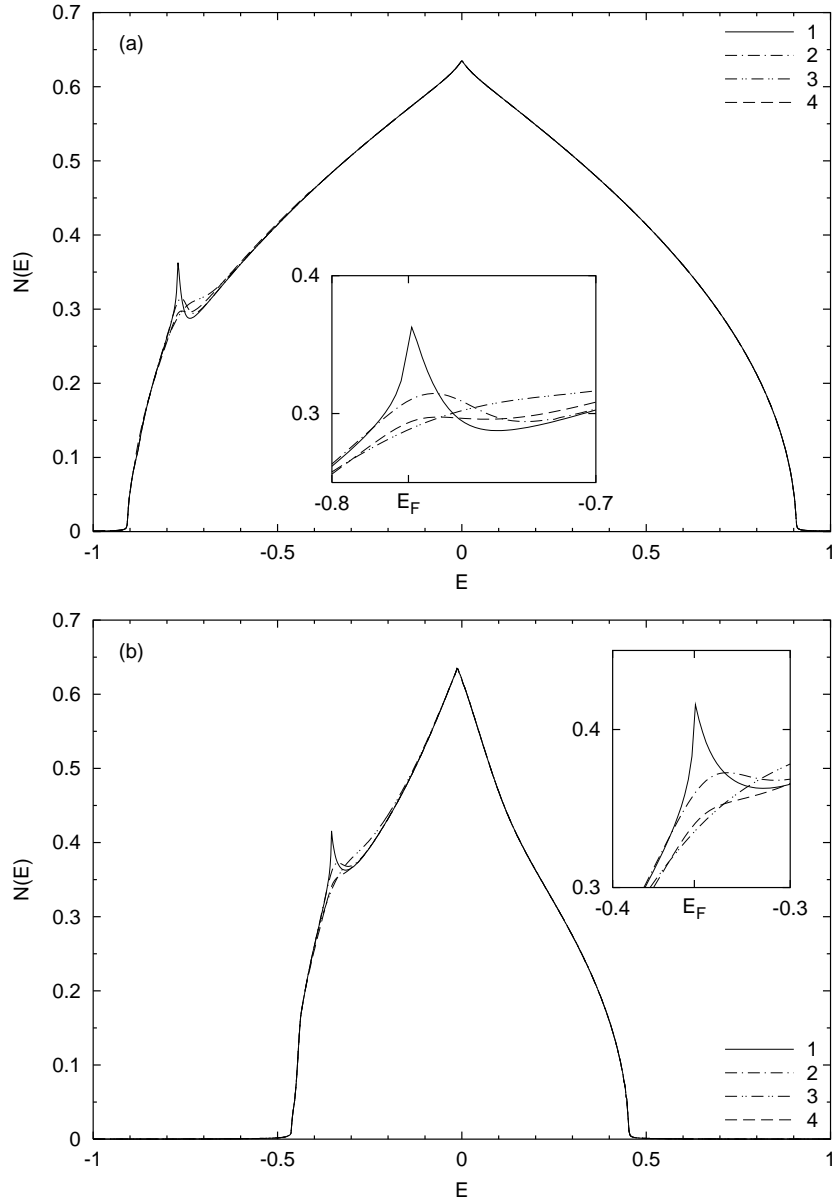
in the complex plane. This can result in the violation of analytical properties, in particular, of the normalization condition

$$L = \langle \{ g_{i\sigma\alpha}, g_{i\sigma\alpha}^\dagger \} \rangle = P_\alpha \qquad (13)$$

where

$$L \equiv \int\limits_{-\infty}^{+\infty} dE N_\alpha(E).$$

The analytical properties turn out to be different for the cases of positive and negative I. For $I > 0$ the singularity lies in the upper half-plane, and for $I < 0$ in the lower

Fig. 3. The density of states picture in the self-consistent approximation (15) for $S = 1/2$, $n = 0.05$.

one, so that the normalization condition is violated for $I < 0$, although this violation is numerically not too large (see Tab. 1). This difficulty does not seem to lead to unphysical conclusions in our simple approximation, since the results for the DOS picture in both the cases are qualitatively similar. However, it should be stressed that this problem has a rather general character and is typical for most calculations which use the many-electron Hubbard representation (or related slave-boson and slave-fermion representations which include constraint conditions). It is connected with the **k**-dependence of "perturbation" (band energy $t_{\mathbf{k}}$), which changes its sign in the band, and a complicated structure of the Green's function (the simple Dyson equation is not valid). By these reasons, the signs of the corresponding imaginary parts are not fixed; the

problems increase when using self-consistent procedures. In particular, such a difficulty should occur in the non-crossing approximation (NCA) for the Anderson model where an expansion in the hybridization $V_{\mathbf{k}}$ is constructed. Unfortunately, this problem is usually misregarded since the normalization condition is practically never verified.

The approximation (6, 7, 8) has an unpleasant physical drawback: DOS has the "Van Hove" singularities at the energies, corresponding to the edges of the Hubbard-I band [5]. To remove this drawback, we renormalize self-consistently the bandwidths in the resolvents (*i.e.*, in the denominators in (10, 11)) and in the Fermi functions by replacing

$$E - P_\alpha t_{\mathbf{k}-\mathbf{q}} \rightarrow E - \widetilde{P}_\alpha t_{\mathbf{k}-\mathbf{q}}. \tag{14}$$

Table 1. Values of the normalization factors L/P_α (see Eq. (13)) for semielliptic bare DOS in (I) the approximation (7, 8); (II) the self-consistent approximation (14); (III) the self-consistent approximation (15).

α	n	L/P_α		
		I	II	III
$+$	0.20	1.000	1.000	1.022
$+$	0.15	1.000	1.000	1.017
$+$	0.10	1.000	1.000	1.011
$+$	0.05	1.000	1.000	1.004
$+$	0.02	1.000	1.000	1.002
$+$	0.00	1.000	1.000	1.001
$-$	0.00	1.510	1.395	1.325
$-$	0.02	1.489	1.366	1.328
$-$	0.05	1.448	1.337	1.318
$-$	0.10	1.385	1.331	1.277
$-$	0.15	1.342	1.246	1.227
$-$	0.20	1.289	1.192	1.177

Due to this self-consistency procedure, the band edges in the resolvents coincide with those for the total Green's function (6). The corresponding numerical results are shown in Figure 2. The analytical properties for $I > 0$ are not violated (Tab. 1). This approximation is in spirit of large-N expansion and retains the quasiparticle picture, unlike the Hubbard-III approximation and the self-consistent approximation considered below which yield a strongly incoherent behavior.

Finally, we discuss also the "true" self-consistent approximation where the exact Green's functions are included into resolvents. Then we have to replace in the denominators of (10, 11)

$$E - P_\alpha t_{\mathbf{k-q}} \rightarrow b_{\mathbf{k-q}\alpha}(E) - a_{\mathbf{k-q}\alpha}(E)t_{\mathbf{k-q}} \qquad (15)$$

and to make the corresponding renormalization of the distribution functions

$$n_{\mathbf{k}\alpha} = -\frac{1}{\pi} \int \mathrm{d}E f(E) \operatorname{Im} G_{\mathbf{k}\alpha}(E).$$

One can see that the DOS picture (Fig. 3) becomes somewhat smeared even in the absence of spin dynamics, but the smearing is not so strong as in the FM case [10].

In this self-consistent approximation, the analytical properties are violated for both $I > 0$ and $I < 0$ (Tab. 1).

To conclude, we have analyzed formation of the "Kondo" peak in narrow-band systems at the Fermi level within a simple analytical approach. The numerical results demonstrate sharp energy dependence of the density of states near E_F. As well as in the standard Kondo problem, one can expect strong temperature dependences of thermodynamic and transport properties (*e.g.*, an enhancement of the effective electron mass). This problem needs further investigations. In particular, summation of higher-order perturbation corrections with the use of slave boson and fermion representations would be of interest.

References

1. A. Georges, G. Kotliar, Phys. Rev. B **45**, 6479 (1993); X.Y. Zhang, C.M. Zhang, Phys. Rev. B **49**, 7929 (1994); M.J. Rozenberg, G. Kotliar, X.Y. Zhang, Phys. Rev. B **49**, 10181 (1994); F.J. Ohkawa, J. Phys. Soc. Jpn **61**, 1615 (1992).
2. A. Georges, G. Kotliar, W. Krauth, M.J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
3. V.I. Anisimov, A.I. Poteryaev, M.A. Korotin, A.O. Anokhin, G. Kotliar, J. Phys. Cond. Mat. **9**, 7359 (1997).
4. J. Hubbard, Proc. Roy. Soc. A **281**, 401 (1964).
5. A.O. Anokhin, V.Yu. Irkhin, Phys. Stat. Sol. b **165**, 129 (1991).
6. A.O. Anokhin, V.Yu. Irkhin, M.I. Katsnelson, J. Phys. Cond. Mat. **3**, 1475 (1991).
7. J. Hubbard, Proc. Roy. Soc. A **285**, 542 (1965).
8. V.Yu. Irkhin, Yu.P. Irkhin, Phys. Stat. Sol. b **183**, 9 (1994).
9. M.Sh. Erukhimov, S.G. Ovchinnikov, Phys. Stat. Sol. b **123**, 105 (1984); V.Yu. Irkhin, M.I. Katsnelson, Zh. Eksp. Teor. Fiz. **88**, 522 (1985); V.Yu. Irkhin, M.I. Katsnelson, J. Phys. C **18**, 4173 (1985).
10. A.V. Zarubin, V.Yu. Irkhin, Fiz. Tverd. Tela **41**, 1057 (1999) [Phys. Solid State, **41**, 963 (1999)].
11. V.Yu. Irkhin, M.I. Katsnelson, Z. Phys. B **75**, 67 (1989).
12. V.Yu. Irkhin, M.I. Katsnelson, J. Phys. Cond. Mat. **2**, 8715 (1990).