Single-site Anderson model. II Perturbation theory of symmetric model

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The strong electron correlations caused by Coulomb interaction of impurity electrons are taken into account. The infinite series of diagrams containing irreducible Green's functions are summed. For symmetric Anderson model we establish the antisymmetry property of the impurity Green's function, formulate the exact Dyson type equation for it, find the approximate correlation function $Z_\sigma(i\omega)$ and solve the integral equation which determines the full propagator of the impurity electrons. Analytical continuation of the obtained Matsubara Green's function determines the retarded one and gives the possibility to find the spectral function of impurity electrons. The existence of two resonances of this function has been proved. The smooth behaviour was found near the Fermi surface. The two resonances situated symmetrical to the Fermi surface correspond to the energies of quantum transitions of the impurity electrons. The widths and heights of these resonances are established.

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I. INTRODUCTION

We shall investigate the properties of the normal state of single-site Anderson model. For that we shall use the results of diagrammatic theory for this model developed in our previous paper[1]. In that investigation the notion of irreducible Green's function has been introduced. These functions contain the main spin, charge and pairing fluctuations caused by the strong Coulomb repulsion of impurity electrons. We have determined the notion of correlation function $Z_{\sigma\sigma'}$ as composed from strong connected diagrams containing the irreducible Green's functions. In superconducting state of the system there are additional correlation functions $Y_{\sigma\sigma'}$ and $\overline{Y}_{\overline{\sigma}\sigma'}$ which are the order parameters of the system. The correlation functions are the main elements of the Dyson type equations for one–particle renormalized Green's function of conducting and impurity electrons. We shall restrict ourselves only by the discussion of the properties of the normal phase of the system and determine the corresponding Green's functions of conduction and impurity electrons:

$$\begin{aligned} G_{\sigma\sigma'}(\mathbf{k},\tau|\mathbf{k}',\tau') &= -\left\langle T C_{\mathbf{k}\sigma}(\tau)\overline{C}_{\mathbf{k}'\sigma'}(\tau')U(\beta)\right\rangle_0^c, \\ g_{\sigma\sigma'}(\tau|\tau') &= -\left\langle T f_\sigma(\tau)\overline{f}_{\sigma'}(\tau')U(\beta)\right\rangle_0^c, \end{aligned} \tag{1}$$

where index "c" means connected.

Fourier representation is denoted as $G_{\sigma\sigma'}(\mathbf{k},\mathbf{k}'|i\omega)$ and $g_{\sigma\sigma'}(i\omega)$ correspondingly. For these two functions we have obtained the results[1] :

$$\begin{aligned} G_\sigma(\mathbf{k},\mathbf{k}'|i\omega) &= \delta_{\mathbf{k}\mathbf{k}'}G^0_\sigma(\mathbf{k}|i\omega) + \frac{V_{\mathbf{k}}V^*_{\mathbf{k}'}}{N}G^0_\sigma(\mathbf{k}|i\omega)g_\sigma(i\omega)G^0_\sigma(\mathbf{k}'|i\omega), \\ g_\sigma(i\omega) &= \frac{\Lambda_\sigma(i\omega)}{1-\Lambda_\sigma(i\omega)G^0_\sigma(i\omega)}, \\ \Lambda_\sigma(i\omega) &= g^0_\sigma(i\omega) + Z_\sigma(i\omega), \end{aligned} \tag{2}$$

where zero order propagators of the conduction and impurity electrons have the form ($\overline{\sigma} = -\sigma$).

$$\begin{aligned} G^0_\sigma(\mathbf{k}|i\omega) &= (i\omega - \epsilon(\mathbf{k}))^{-1}, \\ g^0_\sigma(i\omega) &= \frac{1-n_{\overline{\sigma}}}{i\omega-\epsilon_f} + \frac{n_{\overline{\sigma}}}{i\omega-\epsilon_f-U}, \end{aligned}$$

$$\begin{aligned} n_{\overline{\sigma}} &= \frac{\exp(-\beta\epsilon_f) + \exp\left[-\beta(2\epsilon_f+U\right]}{Z_0}, \\ Z_0 &= 1 + 2\exp(-\beta\epsilon_f) + \exp\left[-\beta(2\epsilon_f+U\right], \\ G^0_\sigma(i\omega) &= \frac{1}{N}\sum_{\mathbf{k}}|V_{\mathbf{k}}|^2 G^0_\sigma(\mathbf{k}|i\omega) = \int\frac{V^2(\epsilon)\rho_0(\epsilon)d\epsilon}{i\omega-\epsilon}. \end{aligned} \tag{3}$$

Here $\epsilon(\mathbf{k})$ is the energy of conduction band and ϵ_f of local impurity electrons, $\rho_0(\epsilon)$ is the density of states of the bare conduction band and matrix element of hybridization $V_{\mathbf{k}}$ is supposed dependent of the energy. U is Coulomb repulsion of the impurity electrons. $\omega \equiv \omega_n = (2n+1)\pi/\beta$ is odd Matsubara frequency. The equations (2) are exact, but for correlation function $Z_\sigma(i\omega)$ doesn't exist exact Dyson type equation and only the approximate contribution can be available: see *Fig.* 9 of paper[1]. Our main approximation formulated in paper[1] comes to the summation of the ladder diagrams which will be enough to obtain the main contributions of the spin and charge fluctuations. This approximation has used only the simplest irreducible Green's function $g_2^{(0)ir}$ which is iterated many times. It has the form:

$$Z_{\sigma\sigma'}(\tau-\tau^{'}) \;=\; -\sum_{\mathbf{k}_1\mathbf{k}_2\sigma_1\sigma_2}\int_0^\beta d\tau_1\int_0^\beta d\tau_2 g_2^{(0)ir}[\sigma,\tau;\sigma_1,\tau_1|\sigma_2,\tau_2;\sigma',\tau']\frac{1}{N}V^*_{\mathbf{k}_1}V_{\mathbf{k}_2}G_{\sigma_2\sigma_1}(\mathbf{k}_2,\tau_2|\mathbf{k}_1,\tau_1), \tag{4}$$

or in Fourier representation

$$Z_{\sigma\sigma'}(i\omega) \;=\; -\frac{1}{\beta}\sum_{\omega_1}\sum_{\sigma_1\sigma_2}\sum_{\mathbf{k}_1\mathbf{k}_2}\widetilde{g}_2^{(0)ir}[\sigma,i\omega;\sigma_1,i\omega_1|\sigma_2,i\omega_1;\sigma',i\omega]\frac{1}{N}V^*_{\mathbf{k}_1}V_{\mathbf{k}_2}G_{\sigma_2\sigma_1}(\mathbf{k}_1,\mathbf{k}_2|i\omega_1). \tag{5}$$

Here we take into account the conservation law of the frequencies:

$$g_2^{(0)ir}[\sigma,i\omega;\sigma_1,i\omega_1|\sigma_1,i\omega_1;\sigma',i\omega'] \;=\; \beta\delta(\omega-\omega')\widetilde{g}_2^{(0)ir}[\sigma,i\omega;\sigma_1,i\omega_1|\sigma_2,i\omega_1;\sigma',i\omega]. \tag{6}$$

In paramagnetic phase we have more simple equation ($\sigma'=\sigma$):

$$Z_\sigma(i\omega) \;=\; -\frac{1}{\beta}\sum_{\omega_1}\sum_{\sigma_1}\widetilde{g}_2^{(0)ir}[\sigma,i\omega;\sigma_1,i\omega_1|\sigma_1,i\omega_1;\sigma,i\omega]G_{\sigma_1}(i\omega_1), \tag{7}$$

where

$$G_\sigma(i\omega) = \frac{1}{N}\sum_{\mathbf{k}_1\mathbf{k}_2}V^*_{\mathbf{k}_1}V_{\mathbf{k}_2}G_\sigma(\mathbf{k}_1,\mathbf{k}_2|i\omega). \tag{8}$$

On the base of equations (2) and (3) the last function (8) can be presented in the form:

$$G_\sigma(i\omega) = G^0_\sigma(i\omega)+[G^0_\sigma(i\omega)]^2 g_\sigma(i\omega) = \frac{G^0_\sigma(i\omega)}{1-\Lambda_\sigma(i\omega)G^0_\sigma(i\omega)}. \tag{9}$$

By using the definition (2) of correlation function of normal state $\Lambda_\sigma(i\omega)$ and approximation (7) for function $Z_\sigma(i\omega)$, we obtain the final integral equation for Λ_σ:

$$\Lambda_\sigma(i\omega) = g^{(0)}_\sigma(i\omega) - \frac{1}{\beta}\sum_{\omega_1}\sum_{\sigma_1}\widetilde{g}_2^{(0)ir}[\sigma,i\omega;\sigma_1,i\omega_1|\sigma_{1,}i\omega_1;\sigma,i\omega]\frac{G^0_{\sigma_1}(i\omega_1)}{1-\Lambda_{\sigma_1}(i\omega_1)G^0_{\sigma_1}(i\omega_1)}. \tag{10}$$

In the second Section of this paper we shall discuss the simplest case of symmetric impurity Anderson model with the condition $2\epsilon_f+U=0$. In Section III the spectral function of the impurity electrons is analyzed and the last Section IV contains the conclusions.

II. SYMMETRIC MODEL

In symmetric case when $\epsilon_f = -U/2 < 0$ and $\epsilon_f + U = U/2 > 0$ we have more simple equations:

$$g^0_\sigma(i\omega) \;=\; \frac{i\omega}{(i\omega)^2-(U/2)^2},$$