ON THE METHOD OF ORTHOGONAL OPERATORS IN THE PROBLEM OF DILUTE ALLOYS

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The method of orthogonal operators is applied to the generalized Anderson Hamiltonian in order to find the one-particle Green function of impurity electrons. In the limiting case of orthogonal representation Roth's result for the Anderson model is obtained. For the case of full non-orthogonality the solution of the Wolff model corresponding to the result of Roth for the Anderson model is derived.

1. Introduction

There are two different approaches to the problem of the formation of the localized magnetic moments in dilute alloys: one proposed by Anderson [1], the other by Wolff [2]. The local moment formation in the Anderson model has been studied extensively beyond the Hartree-Fock approximation [3, 4]. Due to mathematical difficulties only recently the Wolff model has been discussed from such a point of view [5]. Here we want to present the application of the method of orthogonal operators [6] to the more general Hamiltonian for which the Anderson and Wolff models are the limiting cases. The Hamiltonian is of the form

$$H = \sum_{k,\sigma} \varepsilon_k c_{k\sigma}^+ c_{k\sigma} + E \sum_{\sigma} a_\sigma^+ a_\sigma + \frac{V}{\sqrt{N}} \sum_{k,\sigma} c_{k\sigma}^+ a_\sigma + a_\sigma^+ c_{k\sigma} + U a_\uparrow^+ a_\uparrow a_\downarrow^+ a_\downarrow \tag{1}$$

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and the anticommutation rules between impurity a_σ and conduction electrons $c_{k\sigma}$ operators are

$$\{a_\sigma, c^+_{k\sigma'}\} = \frac{1}{\sqrt{N}}\mu\delta_{\sigma\sigma'}, \qquad \{a_\sigma, c_{k\sigma'}\} = 0. \tag{2}$$

For $\mu = 0$ we get the usual Anderson Hamiltonian in orthogonal representation and for $\mu = 1$ the Wolff model with the scattering potential $2V+E$ is obtained. In the first case the impurity is represented by the extra orbital and in the second one the impurity orbital is the composition of the band state only. Since we are interested in these two limiting cases here, we shall not discuss the problem of the $\boldsymbol{k}$ independence of μ [7]. To investigate the Hamiltonian (1) the standard method of equations of motion for the anticommutator Green functions will be used [8]. The Fourier-transformed Green function will be denoted by $\langle\langle A|B\rangle\rangle$ nad $\langle\ldots\rangle$ will stand for the thermal average. The notation $a^+_\sigma a_\sigma \equiv n_\sigma$ for the impurity electrons number operator ($\sigma = \uparrow, \downarrow$) is also introduced.

2. *Calculations and results*

We are interested in the one-particle Green function for impurity electrons. The following system of equations of motion is derived

$$(\omega-E)\langle\langle a_\sigma|a^+_\sigma\rangle\rangle = 1+\mu V\langle\langle a_\sigma|a^+_\sigma\rangle\rangle+\frac{V}{\sqrt{N}}\sum_k\langle\langle c_{k\sigma}|a^+_\sigma\rangle\rangle$$

$$+\frac{\mu}{\sqrt{N}}\sum_k\varepsilon_k\langle\langle c_{k\sigma}|a^+_\sigma\rangle\rangle+U\langle\langle a_\sigma n_{-\sigma}|a^+_\sigma\rangle\rangle, \tag{3}$$

$$(\omega-\varepsilon_k)\langle\langle c_{k\sigma}|a^+_\sigma\rangle\rangle = \frac{\mu}{\sqrt{N}}+\frac{1}{\sqrt{N}}(V+\mu E)\langle\langle a_\sigma|a^+_\sigma\rangle\rangle$$

$$+\frac{V\mu}{N}\sum_k\langle\langle c_{k\sigma}|a^+_\sigma\rangle\rangle+\frac{\mu U}{\sqrt{N}}\langle\langle a_\sigma n_{-\sigma}|a^+_\sigma\rangle\rangle, \tag{4}$$

$$(\omega-E-U-\mu V)\langle\langle a_\sigma n_{-\sigma}|a^+_\sigma\rangle\rangle = \langle n_{-\sigma}\rangle+\frac{1}{\sqrt{N}}\sum_k(V+\mu\varepsilon_k)\langle\langle a_\sigma a^+_{-\sigma}c_{k,-\sigma}|a^+_\sigma\rangle\rangle$$

$$-\frac{1}{\sqrt{N}}\sum_k(V+\mu\varepsilon_k)\langle\langle a_\sigma c^+_{k,-\sigma}a_{-\sigma}|a^+_\sigma\rangle\rangle+\frac{1}{\sqrt{N}}\sum_k(V+\mu\varepsilon_k)\langle\langle c_{k\sigma}n_{-\sigma}|a^+_\sigma\rangle\rangle. \tag{5}$$

The new functions which appear in (5) should be expressed approximately in terms of those standing on the left-hand side of (3) to (5). Thus, the operators $A_{1\sigma} = a_\sigma a^+_{-\sigma}c_{k,-\sigma}$, $A_{2\sigma} = a_\sigma c^+_{k,-\sigma}a_{-\sigma}$, $A_{3\sigma} = c_{k\sigma}n_{-\sigma}$ should be expressed in terms of a_σ, $c_{k\sigma}$, $a_\sigma n_{-\sigma}$. We can treat the operators $A_{i\sigma}$ as the elements of Hilbert space $\tilde{\mathscr{H}}$ in which the scalar product is defined by [6]

$$(A, B) \equiv \langle\{A, B^{+}\}\rangle, \quad A, B \in \tilde{\mathscr{H}}. \tag{6a}$$

Let us consider $\tilde{\tilde{\mathscr{H}}} \subset \tilde{\mathscr{H}}$ which is spanned on the set of orthogonalized operators $\{O_i\}$ ($i = 1, \ldots, N$). Then an arbitrary operator $A \in \tilde{\mathscr{H}}$ can be given by the linear combination

$$A = \sum_{i=1}^{N} \alpha_i O_i + B, \tag{6b}$$

where $\alpha_i = (A, O_i)$ and B belongs to the orthogonal complement of $\tilde{\tilde{\mathscr{H}}}$. In our case we have the set of operators $A_{i\sigma}$ which we want to express in terms of those forming the Green functions on the left-hand sides of (3) to (5). In our approximation we neglect the Green functions formed by type B operators as given in (6b). Thus, the set a_σ, $c_{k\sigma}$, $a_\sigma n_{-\sigma}$ can be orthonormalized in the sense of (6a), i. e. it can be replaced by

$$a_{1\sigma} = a_\sigma, \quad a_{2\sigma} = \left(c_{k\sigma} - \frac{\mu}{\sqrt{N}} a_\sigma\right)\left(1 - \frac{\mu^2}{N}\right)^{-1/2}, \tag{7}$$

$$a_{3\sigma} = (a_\sigma n_{-\sigma} - \langle n_{-\sigma}\rangle a_\sigma)\,[\langle n_{-\sigma}\rangle\,(1 - \langle n_{-\sigma}\rangle)]^{-1/2} \tag{8}$$

and the desired expansion can be obtained:

$$A_{1\sigma} = \langle a^{+}_{-\sigma} c_{k,-\sigma}\rangle a_\sigma$$
$$+[\langle n_{-\sigma}\rangle\,(1-\langle n_{-\sigma}\rangle)]^{-1/2}\left[\langle n_\sigma a^{+}_{-\sigma} c_{k,-\sigma}\rangle - \langle n_{-\sigma}\rangle\,\langle a^{+}_{-\sigma} c_{k,-\sigma}\rangle + \frac{\mu}{\sqrt{N}}\langle n_\sigma n_{-\sigma}\rangle\right] a_{3\sigma}, \tag{9}$$

$$A_{2\sigma} = \langle c^{+}_{k,-\sigma} a_{-\sigma}\rangle a_\sigma$$
$$+[\langle n_{-\sigma}\rangle\,(1-\langle n_{-\sigma}\rangle)]^{-1/2}\left[\langle a_\sigma c^{+}_{k,-\sigma} a_{-\sigma} a^{+}_\sigma\rangle + \frac{\mu}{\sqrt{N}}\langle n_\sigma n_{-\sigma}\rangle - \langle n_{-\sigma}\rangle\,\langle c^{+}_{k,-\sigma} a_{-\sigma}\rangle\right] a_{3\sigma}, \tag{10}$$

$$A_{3\sigma} = \langle n_{-\sigma}\rangle c_{k\sigma} + \frac{\mu}{\sqrt{N}}\,[\langle n_{-\sigma}\rangle\,(1-\langle n_{-\sigma}\rangle)]^{1/2} a_{3\sigma}. \tag{11}$$

The substitution of (9)–(11) to the corresponding Green functions in (5) enables us to find

$$\langle\langle a_\sigma | a^{+}_\sigma\rangle\rangle = \frac{T_{-\sigma}(1 + VH_{1,-\sigma} + \mu K_{1,-\sigma})}{\omega - E - \mu V + U_{-\sigma} B_{-\sigma} - T_{-\sigma}(VH_{2,-\sigma} + \mu K_{2,-\sigma})}, \tag{12}$$

where

$$T_\sigma = (1 + U_\sigma\langle n_\sigma\rangle), \tag{13}$$

$$H_{1\sigma} = \mu F U_\sigma P_\sigma, \quad H_{2\sigma} = F V_\sigma P_\sigma, \quad K_{1\sigma} = \mu L U_\sigma P_\sigma, \quad K_{2\sigma} = L V_\sigma P_\sigma, \tag{14}$$

$$P_\sigma = 1 - \mu^2 U_\sigma \langle n_\sigma\rangle L - \mu V F T_\sigma, \tag{15}$$

$$U_\sigma = U M_\sigma^{-1}, \quad V_\sigma = V + \mu E - \mu U_\sigma B_\sigma, \tag{16}$$

$$M_\sigma = \omega - E - U - 2\mu V - W_\sigma - \mu Z_\sigma - \frac{\mu^2}{N}\sum_k \varepsilon_k, \tag{17}$$

$$B_\sigma = \langle n_\sigma \rangle \left(W_\sigma + \mu V + \mu Z_\sigma + \frac{\mu^2}{N}\sum_k \varepsilon_k \right), \tag{18}$$

$$F = \frac{1}{N}\sum_k \frac{1}{\omega - \varepsilon_k}, \qquad L = \omega F - 1, \tag{19}$$

$$W_\sigma \langle n_\sigma \rangle (1 - \langle n_\sigma \rangle) = -\frac{V}{\sqrt{N}}\sum_k \Theta_{k\sigma}, \qquad Z_\sigma \langle n_\sigma \rangle (1 - \langle n_\sigma \rangle) = -\frac{1}{\sqrt{N}}\sum_k \varepsilon_k \Theta_{k\sigma}, \tag{20}$$

$$\Theta_{k\sigma} = \langle c_{k\sigma}^{+} a_\sigma (1 - 2a_{-\sigma}^{+} a_{-\sigma}) \rangle + \frac{2\mu}{\sqrt{N}} \langle n_\sigma n_{-\sigma} \rangle - \frac{\mu}{\sqrt{N}} \langle n_\sigma \rangle. \tag{21}$$

In the limiting case $\mu = 0$ we get the result of Roth [4]

$$\langle\langle a_\sigma | a_\sigma^{+} \rangle\rangle = \frac{\omega - E - W_{-\sigma} - U(1 - \langle n_{-\sigma} \rangle)}{(\omega - E - V^2 F)(\omega - E - U - W_{-\sigma}) - U \langle n_{-\sigma} \rangle (V^2 F - W_{-\sigma})} \tag{22}$$

and when $\mu = 1$, the solution of the Wolff model with the scattering potential $2V+E$ is obtained

$$\langle\langle a_\sigma | a_\sigma^{+} \rangle\rangle = \frac{F}{1 - D_{-\sigma} F}, \tag{23}$$

where

$$D_\sigma = \frac{(2V+E)N_\sigma + U\langle n_\sigma \rangle \left(\omega - Z_\sigma - \frac{1}{N}\sum_k \varepsilon_k \right)}{N_\sigma + U \langle n_\sigma \rangle}, \tag{24}$$

$$N_\sigma = \omega - E - 2V - U - Z_\sigma - \frac{1}{N}\sum_k \varepsilon_k. \tag{25}$$

In (25) Z_σ as given by (20) and (21) for $\mu = 1$ is understood. It can be checked that for the case $\mu = 1$ the equality

$$\frac{1}{\sqrt{N}}\sum_k \langle\langle c_{k\sigma} | a_\sigma^{+} \rangle\rangle = \langle\langle a_\sigma | a_\sigma^{+} \rangle\rangle \tag{26}$$

holds, as should be due to the fact that the impurity orbital is constructed from the band ones.

It must be noted that $\langle n_\sigma \rangle$ cannot be calculated with the use of Eq. (22) or (23) only. The correlation functions which appear in W_σ or Z_σ should be calculated from corresponding Green functions. We have obtained

$$\langle\langle a_\sigma n_{-\sigma} | a_\sigma^+ \rangle\rangle = M_{-\sigma}^{-1} \Big\{ \langle n_{-\sigma} \rangle - B_{-\sigma} \langle\langle a_\sigma | a_\sigma^+ \rangle\rangle + \frac{V}{\sqrt{N}} \langle n_{-\sigma} \rangle \sum_k \langle\langle c_{k\sigma} | a_\sigma^+ \rangle\rangle + \frac{\mu}{\sqrt{N}} \langle n_{-\sigma} \rangle \sum_k \varepsilon_k \langle\langle c_{k\sigma} | a_\sigma^+ \rangle\rangle \Big\} \tag{27}$$

and

$$\frac{1}{\sqrt{N}} \sum_k \langle\langle c_{k\sigma} | a_\sigma^+ \rangle\rangle = H_{1,-\sigma} + H_{2,-\sigma} \langle\langle a_\sigma | a_\sigma^+ \rangle\rangle, \tag{28}$$

$$\frac{1}{\sqrt{N}} \sum_k \varepsilon_k \langle\langle c_{k\sigma} | a_\sigma^+ \rangle\rangle = K_{1,-\sigma} + K_{2,-\sigma} \langle\langle a_\sigma | a_\sigma^+ \rangle\rangle. \tag{29}$$

Eq. (10) accomplishes the systems of Green functions needed to be known for the selfconsistent calculation of $\langle n_\sigma \rangle$. It must be noted that for the case of the Wolff model ($\mu = 1$) this set can be simplified only when $u \to \infty$ (even for the case of symmetric band, $\frac{1}{N} \sum_k \varepsilon_k = 0$). Then $\langle\langle a\, n^- \, | a^+ \rangle\rangle = 0$ which is visible from (27).

3. *Summary*

We have applied the method of orthogonal operators to the calculation of the one--particle Green function of impurity electrons for the generalized Hamiltonian for which the Anderson and Wolff models are the limiting cases. Such a formulation enables one to treat both models with the same accuracy within the framework of a given mathematical method. We have got the result of Roth for the Anderson model and the corresponding solution for the Wolff model in simple manner. It is also worthy to mention the possibility of further improvement. In order to obtain Kondo-type effects one must enlarge the set of orthonormal operators (7) and (8) to include those appearing in decoupled Green functions in (5). Usually, the equations of motion for these Green functions are decoupled in terms of $\langle\langle a_\sigma | a_\sigma^+ \rangle\rangle$ and $\langle\langle c_{k\sigma} | a_\sigma^+ \rangle\rangle$ [10]. Such an approximation leads to the spurious solution for the case $2E + U = 0$ in the Anderson model [11]. From our point of view this corresponds to the neglecting of all the orthonormal operators in (6b) except of a_σ and $c_{k\sigma}$, which seems to be a rough approximation. Instead of this the above mentioned enlarged set should be considered. The presented method does not lead to the enormous mathematical difficulties in the case of such an enlarged set, in contrast to the Roth's approach. It is an interesting problem for further research.

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