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PARTIAL CANCELLATION IN THE ELECTRON-HOLE AND ELECTRON-ELECTRON CORRELATION IN THE SYMMETRIC ANDERSON MODELL

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ABSTRACT

We show that there is a symmetry transformation in the symmetric Anderson model which consist of an electron-hole transformation applied only for one spin-direction and the change of sign of the Coulomb energy U. By using this symmetry it is possible to prove that both the electron-electron and electron-hole correlation are of importance and several quantities must be even function in U in the localized spin fluctuation theory.

KIVONAT

Megmutatjuk, hogy a szimmetrikus Anderson modell esetében van egy olyan szimmetria-transzformáció, amely csupán az egyik spin állásu elektronokra alkalmazott elektron-lyuk transzformációból és az U Coulomb energia előjelének megváltoztatásából áll. Felhasználva ezt a transzformációt bebizonyitjuk, hogy a lokalizált spin fluktuáció-modellben az elektron-elektron és az elektron-lyuk korrelációk egyaránt lényegesek és több különböző mennyiség U páros függvénye.

РЕЗЮМЕ

В статье показано, что в симметрической модели Андерсона существует преобразование симметрии, которое содержит электронно-дырочное преобразование, примененное только для одного из спиновых направлений и изменение знака кулоновской энергии. С помощью этого преобразования доказывается, что в модели локализированной спиновой флюктуации как электронно-электронные, так и электронно-дырочные корреляции - значительны, и несколько из величин являются четными функциями кулоновской энергии.

Since long time the nondegenerate Anderson model[1] has provided the base for studying the properties of one impurity in non-magnetic host. In the treatment of this model the crucial problem is how to handle the Coulomb repulsion between two electrons with opposite spins on the localized orbital. This problem has been attacked on two different lines depending whether the electron-electron or the electron-hole correlation has been assumed to be the dominating one. The first case has been worked out by Schrieffer and Mattis[2] who emphasized that the electron-hole correlation can be neglected only in case of low electron /or hole/ density, where for the occupation of the localized orbital by spin-up and spin-down electrons holds

$$\frac{\langle n_{d\uparrow}\rangle + \langle n_{d\downarrow}\rangle}{2} \ll 1 \quad \text{or} \quad 1 - \frac{\langle n_{d\uparrow}\rangle + \langle n_{d\uparrow}\rangle}{2} \ll 1$$

respectively, as it is known since the early days of the many body theory[3]. Nevertheless, five years ago Suhl has suggested that in the opposite case it is sufficient to consider only the electron-hole correlation[4,5] and this idea has been followed by several authors[6,7,8] working on the localized-spin fluctuation /LSF/ model. In the following one of the most favorite limits of this model the symmetric case will be discussed.

The aim of the present letter is to exploit the consequences of the electron-hole symmetry existing for a special set of parameter values that in the non-magnetic limit the impurity level renormalized in Hartree-Fock approximation and the density of states of the conduction band are symmetric to the Fermi energy. It is important to notice that using such parameters of the model our considerations are not restricted to the non-magnetic case, but hold for the magnetic case, as well. As it is well known, if one applies the electron-hole symmetry transformation for the conduction electrons and for the localized electrons for both spin orientations simultaneously, then one gets the following symmetry of the scattering amplitude $t^{x}(\omega-i\delta) = -t(-\omega-i\delta)$. We suggest now the application of such transformation only for e.g. spin-up electrons leaving the spin-down electron states unaltered by which one obtains an other physical system. However, in order to achieve a complete symmetry transformation the sign of the Coulomb energy U should be changed, as well. This is obvious, because applying this electron-hole transformation restricted to one spin-direction the repulsion of spin-up and spin-down electrons on the impurity level goes into repulsion between spin-down electron-and hole, which can be remedied by changing the sign of U. This symmetry transformation let us to show that several quantities of the LSF model should be even function of the Coulomb repulsion which may be interpreted as a consequence of the comparable strength of the electron-hole and electron-electron correlation.

The Anderson Hamiltonian can be written as the sum of the following terms

$$H = H_o + H_o' + H_V + H_U \qquad /1/$$

where

$$H_o = \sum_{\lambda s} \left(a^+_{\lambda s}\, a_{\lambda s} + b^+_{\lambda s}\, b_{\lambda s}\right) \qquad /1a/$$

$$H_o' = -\frac{U}{4} + \left(\varepsilon_d + \frac{U}{2}\right)\left(d^+_s\, d_s + d^+_{-s}\, d_{-s}\right) \qquad /1b/$$

$$H_V = \sum_{\lambda s} V_{\lambda d}\, d^+_s\left(a_{\lambda s} + b^+_{\lambda -s}\right) + \text{c.c.} \qquad /1c/$$

$$H_U = U\left(d^+_s\, d_s - \frac{1}{2}\right)\left(d^+_{-s}\, d_{-s} - \frac{1}{2}\right) \qquad /1d/$$

furthermore, a^+_s $/b^+_{-s}/$ is the creation operator of a conduction electron above /or hole below/ the Fermi level with spin s /-s/, similarly d^+_s refers to the electron on the localized level with energy ε_d, and $V_{\lambda d}$ denotes the transition amplitude of a conduction electron to the localized level, finally, U is the Coulomb energy. By introducing the common index λ and energy ε_λ for electrons and holes the electron-hole symmetry is ensured in the conduction band.

Furthermore, we assume a symmetric localized level position to the Fermi level, thus the parameters satisfy the following equation

$$\varepsilon_d + \frac{U}{2} \equiv 0 \qquad /2/$$

so the term given by Eq. (1b) becomes a constant $H_o' = -U/4$.

Now we give the unitary operator of the canonical transformation by which the spin-up electrons and holes are transformed into each other

$$T = \left(d_\uparrow^+ + d_\uparrow\right)\left(1 - a_{\lambda\uparrow}^+ a_{\lambda\uparrow} - b_{\lambda\downarrow}^+ b_{\lambda\downarrow} - a_{\lambda\uparrow}^+ b_{\lambda\downarrow} - b_{\lambda\downarrow}^+ a_{\lambda\uparrow}\right) \qquad /3/$$

This transformation acts on Heisenberg operators taken at time t=0 in the following way

$$T\, a_{\lambda\uparrow}^+(0)\, T^{-1} = -b_{\lambda\downarrow}^+(0)$$

and /4/

$$T\, d_\uparrow^+(0)\, T^{-1} = d_\uparrow(0)$$

while the operators $a_{\lambda\downarrow}^+(0)$, $b_{\lambda\uparrow}^+(0)$ and $d_\downarrow^+(0)$ are invariant.

It is easy to check that this transformation leaves invariant the first three terms of the Hamiltonian given by Eqs. (1a-c), but changes the sign of the Coulomb term given by Eq. (1d), i.e.

$$T\, H_U\, T^{-1} = -\, H_U = H_{-U} \ . \qquad /5/$$

These mean that if one applies this canonical transformation and simultaneously changes the sign of U in H_U the exact results of the theory are unaltered. E.g. if one consideres the statistical average of the product of some operators $A_1(t_1)$, $A_2(t_2)\ldots$ with positive U then this symmetry results in the following identity

$$\langle A_1(t_1) A_2(t_2)\ldots\rangle_U = \frac{\mathrm{Tr}\left(e^{-\beta H}\, e^{iHt_1}\, A_1(0)\, e^{iH(-t_1+t_2)}\, A_2(0)\, e^{-iHt_2}\ldots\right)}{\mathrm{Tr}\ e^{-\beta H}}\, U =$$

$$= \langle \tilde{A}_1(t_1)\, \tilde{A}_2(t_2)\ldots\rangle_{-U} \qquad /6/$$

where we used that the operation Tr is invariant under unitary transformations and subscript U or $-U$ indicates the sign of the Coulomb term in the Hamiltonian, finally, the operator $\tilde{A}_i$ is defined as $\tilde{A}_i(0) = T A_i(0) T^{-1}$. It is worth mentioning that this result is generally valid and is completely independent of that the impurity behaves magnetic or not.

First we apply our results to the thermal energy. Making use of Eqs. (4) and (6) one gets

$$\langle H_o + H_V + H_U \rangle_U = \langle H_o + H_V + H_U \rangle_{-U}$$

and considering the term H_o' given by Eq. (1b) also, one may conclude that the energy can be written in the general form

$$E = \langle H \rangle = \frac{U}{4} + /\text{terms even in } U/ \quad . \qquad /7/$$

This result has been first derived by Yosida and Yamada[9] in the framework of perturbation theory in U for zero temperature, but is has been considered to be valid only in the non-magnetic limit. In our derivation no such restriction has been made. It may be mentioned that the expression of the energy in the Hartree-Fock approximation (assuming the magnetic limit) can not be written in the form proved above[1].

Similar calculation shows that the free energy also exhibits the same structure as given by Eq. (7).

Let us turn to the Green's functions and it will be assumed that in their definitions the average is made with a complete set of states*. Applying the identity given by Eq. (6), e.g. to the down-spin one particle Green's functions. It follows immediately that the one particle Green's function must be an even function of U, thus the self-energy must be an even function, as well

$$\Sigma(\omega)_U = \Sigma(\omega)_{-U} \quad , \qquad /8/$$

e.g. the self-energy of the localized electron must have a vanishing

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* At zero temperature in the magnetic limit some authors[9] define the Green's function as the expectation value of operators taken with one of the two degenerate groundstate wave function. Thus in this case the trace occuring in Eq. (6) does not correspond to a complete set of states, therefore, this identity can not be applied to such Green's functions.

contribution in the third order of perturbation theory. Actually, in third order there are two self-energy diagrams given in Fig. 1., which cancel each other, thus the diagrams containing the electron-electron and electron-hole ladders have opposite signs in any odd-orders of the perturbation theory. However, in any higher odd-order there are more diagrams, but they should be completely canceled, as well.

Finally, we discuss the electron-hole correlation function for which the following identity holds as a consequence of Eqs. (4) and (6)

$$\langle d_{-s}(t)\, d_s^+(t)\, d_s(t')\, d_{-s}^+(t') \rangle_U = \qquad /9/$$

$$= \langle d_{-s}(t)\, d_s(t)\, d_s^+(t')\, d_{-s}^+(t') \rangle_{-U}$$

This indentity means that the electron-electron and electron-hole correlation with total spin zero and one resp. are of the same amplitude in any order of U, but in odd-orders they have opposite signs.

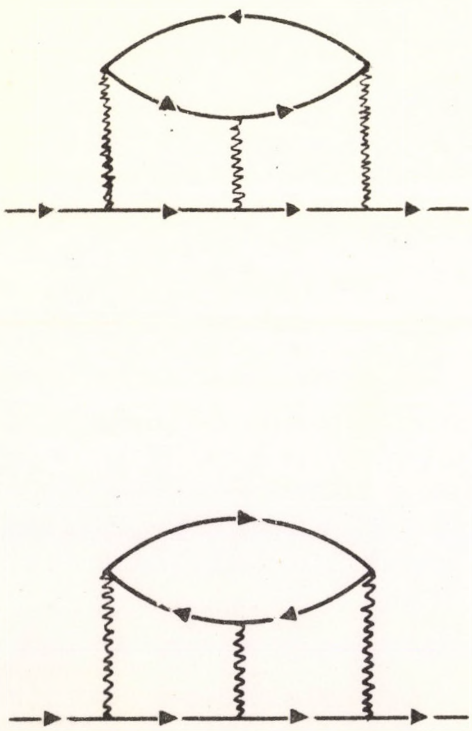

Fig. 1 *Self-energy diagrams in third order of the perturbation theory. The solid and wavy lines represent the propagator of the localized electron and Coulomb interactions, resp.*

The discussion of the applicability of the Schrieffer-Wolff[10] transformation to derive an s-d Hamiltonian could be of considerable interest. However, in the case of the symmetric Anderson model in some approximations[11] where the electron-electron and electron-hole channels were not treated differently it has been found, that some singular contributions cancel each other, therefore, a very careful investigation is required which is beyond the scope of the present paper.

It may be mentioned that similar conclusions may be drawn starting with the other form of the symmetric LSF model suggested by Lederer and Mills[6], but excluding some very special model our results can not be generalized to the problem of the bulk paramagnons. The difficulties arising in this generalization are due to the conservation of the momenta.

Summarizing our results in the case of the symmetric Anderson model the energy and free energy are U/4 and even functions of the Coulomb repulsion. Furthermore, the electron-electron correlation has the same amplitude as the electron-hole correlation in any order of the perturbation theory. This results in the vanishing of the self-energy in odd-orders. One may conclude that in the LSF theory the summation only of the electron-hole ladder diagram is not justified, because e.g. they give finite contribution in odd-orders, as well. Our results on the different correlations given by Eq. (9) strongly suggest that in a correct LSF theory the electron-electron and electron-hole correlations must be treated simultaneously, which means in terms of diagrams the summation of the "parquet" diagrams. To our knowledge until now no succesful attempt has been made on this line. We should emphasize that before a fundamental improvement or clarification of the localized spin fluctuation theories the numerical comparision of the experimental data with theoretical results is meaningless.

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