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SECOND-ORDER U-PERTURBATION SELF-ENERGY FOR HUBBARD HAMILTONIAN: NON-EQUIVALENCE OF THE PHYSICAL AND KOHN-SHAM FERMI SURFACES

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1. Introduction

A central problem in one-electron band calculations is a proper inclusion of the electron correlations. The complete Hamiltonian for a n -body problem is so difficult to handle that simple models have to be developed. The simplest of them, but not trivial, is a Hubbard model which describes a nondegenerate electron band with a local on-site Coulomb interaction /1/. In spite of its simplicity, very few exact results exist in the literature and approximations must be tolerated. One of widely accepted approximations for appropriate values of parameters inherent of the model is the second-order in U (U - on-site Coulomb integral perturbation approach for the self-energy. The range of the parameter U can be extended if one uses a modified second-order perturbation theory described by Bulk and Jelitto^{/2/}. Out of the large number of spplications of the second-order perturbation theory we merely mention few examples. One of them is the already mentioned work by Bulk and Jelitto in which the effect of the band occupation and Coulomb integral on various single-particle properties has been discussed. Next, we mention works by Kleinman and Mednick^{/3/}. Treglia, Ducastelle and Spanjserd^(4,5), Taranko and Taranko⁽⁶⁾, Taranko, Taranko and $\operatorname{Malek}^{/7,8/}$ in which the electron correlation effects have been considered in realistic or model systems (see also^{/9,10/}). At last. we mention works in which the second-order perturbation approach is adopted to Anderson-type Hamiltonians, see Refs. /11,12/

It is evident that in the case of such a wide use of the second-order perturbation formula for the electron self-energy the nearly exact evaluation of this quantity may be very useful. For that reason, in this paper we propose its evaluation according to sufficiently simple formula which is carefully checked by comparison with the Monte-Carlo integration. As a result, one can evaluate the \vec{k} -dependent (three-dimensional case) self-energy without great numerical effort. As an example of practical use of this self-energy calculations, we have shown that the Fermi surface which results from the quasiparticle picture does not exactly reproduce this one resulting from the density-functional theory. Such a comparison was possible only because of the use of the simple method of evaluation of the \vec{k} -dependent self-energy.

In the next section, we give general analytic formulas for the second-order contribution to the self-energy in the Hubbard model and discuss some its symmetry properties. In section 3, we describe a numerical procedure of the exact and approximate evaluation of the self-energy. Section 4 is devoted to the proof that the two Fermi surfaces mentioned above are not mecessarily the same. Section 5 contains conclusions.

2. The second-order self-energy; symmetry properties

The second-order contribution to the self-energy for the Hubbard model reads as (we consider a paramagnetic case):

$$M(\vec{k}, E) = \frac{U^2}{N^2} \sum_{\vec{p} \neq \vec{q}} \frac{f_{\vec{q}} (1 - f_{\vec{k} + \vec{p}})(1 - f_{\vec{q} + \vec{p}}) + (1 - f_{\vec{q}}) f_{\vec{k} + \vec{p}} f_{\vec{q} + \vec{p}}}{E + \epsilon(\vec{q}) - \epsilon(\vec{k} + \vec{p}) - \epsilon(\vec{q} + \vec{p})} \cdot$$
(1)

This formula can be transformed as follows/2,4,7,8/

$$M(\vec{k},E) = U^{2}\sum_{\vec{k}}e^{i\vec{k}\cdot\vec{R}}\int_{\vec{k}}\int_{\vec{$$

where the function $N(\omega_1, \omega_2, \omega_3)$ combines all $f_{\vec{k}}$ factors appearing in Eq.(1). For the temperature $T = 0^{\circ}K$ one obtains

$$M(\vec{k}, E) = U^{2} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{R}} M(\vec{R}, E),$$
 (3)

where

$$M(\vec{R}, E) = \int_{-W}^{E_F} d\omega_1 \int_{E_F}^{W} d\omega_3 \frac{D(\vec{R}, \omega_1)D(\vec{R}, \omega_2)D(\vec{R}, \omega_3)}{E + \omega_1 - \omega_2 - \omega_3} + \int_{E_F}^{W} \int_{E_F}^{E_F} \int_{C_F}^{E_F} \frac{D(\vec{R}, \omega_1)D(\vec{R}, \omega_2)D(\vec{R}, \omega_3)}{E + \omega_1 - \omega_2 - \omega_3} ,$$

$$(4)$$

and $D(\vec{R}, E)$ is "the lattice density of states" connected with the lattice Green function $G_{\vec{n}}(\vec{R}, E)$

$$G(\vec{R}, E) = N^{-1} \sum_{\vec{k}} (E - \epsilon(\vec{k}))^{-1} e^{i\vec{k} \cdot \vec{R}}, \qquad (5)$$

$$D(\vec{R}, E) = -\frac{1}{\pi} \operatorname{Jm} G(\vec{R}, E) = N^{-1} \sum_{\vec{k}} \delta(E - \epsilon(\vec{k})) e^{i \vec{k} \cdot \vec{R}}.$$
 (6)

Here we locate the unperturbed density of states in energy limits (-W, W) and \vec{R} denotes atomic positions in the crystal. In the following we shall consider a simple cubic crystal lattice. Equations (2) and (3) can be further simplified because the lattice density of states $D(\vec{R}, E)$ is the same for all vectors \vec{R}^s connecting the central atom with atoms lying at the same distance from the central one (here ς enumerates

the neighbouring spheres with radius R^{s}). One can obtain (see also /2/)

 $M(\vec{k},E) = U^{2} \sum_{k=1}^{\infty} e(R^{s},\vec{k}) \int \int \int \frac{N(\omega_{1},\omega_{2},\omega_{3})}{E+\omega_{1}-\omega_{2}-\omega_{3}} D(\vec{R}^{s},\omega_{1}) D(\vec{R}^{s},\omega_{3}) D(\vec{R}^{s},\omega_{3}) d\omega_{1} d\omega_{2} d\omega_{3}$ (7) where $\epsilon(\mathbf{R}^{s},\vec{k}) = \sum_{k=1}^{|\vec{R}|=R^{s}} e^{i\vec{k}\cdot\vec{R}}$, $\epsilon(\mathbf{R}^{s},\vec{k})=1$,

 $D(\vec{R},\vec{k}) \equiv D(E)$ is the local density of states and corresponding to the band structure $\epsilon(\vec{k})$. The functions $D(\vec{R}, E)$ are symmetric or antisymmetric functions of the energy depending whether the sum n+l+m is even or odd $^{13/}$. Here, $\vec{R}^{s} = (\vec{l} n + \vec{l} l + \vec{k} m)$ x lattice constant.

In practice, usually the first term of Eqs.(2) or (8) for the self-energy is used /4,5,7,8/, the so-called local approximation. In this case for a half-filled energy band the imaginary part of the self-energy is a symmetric function of the energy and the real part is an antisymmetric function. This can be easily shown. For the imaginary part of Eq.(7) one has

$$Jm M(\vec{k}, E) = -\Pi U^{2} \sum_{s=0}^{\infty} \epsilon(R^{s}, \vec{k}) \iiint_{-\infty} N(\omega_{1}, \omega_{2}, \omega_{3}) D(\vec{R}^{s}, \omega_{1}) D(\vec{R}^{s}, \omega_{2}) \cdot \\ D(\vec{R}^{s}, \omega_{3}) \delta(E + \omega_{1} - \omega_{2} - \omega_{3}) d\omega_{1} d\omega_{2} d\omega_{3} = \\ = -\Pi U^{2} \sum_{s=0}^{\infty} \epsilon(R^{s}, \vec{k}) S(R^{s}, E) , \qquad (8)$$

where $S(R^{s},E) = S(R^{s},-E)$ for $D(\vec{R}^{s},E) = D(\vec{R}^{s},-E)$, (9)

and

$$S(R^{s}_{E}) = -S(R^{s}_{E}-E)$$
 for $D(\vec{R}^{s}_{E}) = -D(\vec{R}^{s}_{E}-E)$.

The symmetry conditions for $S(R^{L}, E)$ can be easily checked for $T = 0^{\circ}K$. In this case (cf. Eq.(4)) one has for a local part. and similarly for other terms (after changing the vari**ables** $\omega_i \rightarrow -\omega_i$)1 $\operatorname{Jm} M(\vec{k}, E) = -\Pi U^2 (\int dw_1 \int dw_2 \int dw_3 +$

$$\int_{-W}^{W} = W \qquad (10)$$

$$+ \int_{-W}^{W} \int_{0}^{W} d\omega_{3} D(\omega_{1}) D(\omega_{2}) D(\omega_{3}) \delta(-E + \omega_{1} - \omega_{2} - \omega_{3}).$$

$$= 0 \qquad \text{Comparing Eq.(10) with the imaginary part of } M(\vec{k}, E) \text{ obtained}$$

from Eq.(4) one has immediately conditions (1). In order to check the symmetry of the self-energy (for a half-filled energy band case) we take

$$Jm M(\vec{k}, E) - Jm M(\vec{k}, E) = -2 \pi U^{2} \sum_{s=1}^{\infty} S(R^{s}, E) e(R^{s}, \vec{k})$$
(11)

where summation is performed over vectors \vec{R}^s for which

m+l+mis odd. Even in the simplest case, i.e. for $\vec{k} = 0$ one obtains

 $\operatorname{Jm} M(0,E) - \operatorname{Jm} M(0,-E) = -2\pi U^2 \left[6 S(R^1,E) + 8 S(R^3,E) + \right]$

+ 24 $S(R^5, E)$ +21 $S(R^8, E)$ +18 $S(R^{10}, E)$ +24 $S(R^{12}, E)$ +...], (12)

i.e. the imaginary part of the self-energy is not a symmetric function of the energy.

3. The second-order self-energy: numerical results

In this section we discuss results of the Monte-Carlo numerical calculations of the second-order self-energy curves and give approximate formulas for fast calculation of this functions. 3.1. Monte-Carlo numerical calculations

Recently we have performed numerical calculation of the second-order self-energy for an extended Hubbard Hamiltonian for SCC and fcc lattices for different band fillings^{6/} and compared with results obtained within the local approximation. The integrals (see Ba. 1) were calculated by using for each \vec{k} -vector about one million random generated pairs of vectors p,q, (or more, for the energy points corresponding to the minima of the corresponding curves). First, we calculated the imaginary part and then obtained the real part by the Kramers--Kronig relation. We have also checked our results by recalculating same curves changing $\vec{k} \rightarrow \vec{k} + \vec{G}$, where G is a reciprocal lattice vector and found that except for variations in the noise, these curves were reproduced. Generally, remarkable differences are observable especially for Γ -points for scc, as well as for fcc lattices. For example, for e scc lattice for a half-filled energy band, the lower minimum of the imaginary part of the self-energy is about 15% deeper then the corresponding one calculated within the local approximation and about 20% deeper for the minimum at higher energies. Additionally, the lower minimum is more narrow then the corresponding one calculated within the local approximation. For others k points the differences are smaller but still significant.

3.2. Lattice Green functions

In this subsection, we give formulas needed for calculation of the lattice densities of states which are required in Eqs. (2,4,7,8,12). The literature on the lattice Greens functions is sufficiently large and we mention here works by G.S.Joyce $^{/14/}$, T.Morita^{/15/}, T.Morita and T.Horiguchi^{/16/} (see also ^{/17/}), Katsura^{/18/}, M.Okazaki et al.^{/19/}, E.Taranko, R.Taranko and M.Pilat^{/20/} and Referencies therein.

We have checked that to obtain a very good agreement between results derived by the Monte-Carlo integration of Eq.(1) and from Eq.(8), one has to take into account the first six terms in the expansion formula (8). For that reason, in our further considerations the lattice Green functions corresponding to S = 0-6 are required and we shortly expound the main ideas concerning calculations of these functions. Not all the lattice Green functions needed for calculation of the self-energy are independent. These functions satisfy the identity

$$\sum_{\vec{s}} G(\vec{n} + \vec{\delta}, E) = \frac{6}{W} \left(\delta_{\vec{n}} \vec{s} - E G(\vec{n}, E) \right), \qquad (13)$$

where $\vec{\delta}$ extends over the six nearest neighbours of the central atom. In our case it is sufficient to obtain the lattice Green functions G(000, E), G(200, E) and G(300, E) from independent calculations and they have been calculated along the way described in Ref.^{/19/}. Other functions, i.e. G(100, E), G(110, E), G(111, E) and G(120, E) can be simply extracted from Eq.(13). In Figs. (1), (2) we depicted the lattice density of states, i.e. $-1/\pi$ Jm G(n(m, E)) and the real part of the lattice Green functions, respectively. We show these functions only for negative values of the energy as they possess the symmetry properties, namely, the real parts are odd or even functions of the energy depending on whether (+m+m) is even or odd (for symmetry of the imaginary part, see the text).



Fig. 1. The "lattice" density of states for different R vectors. For reasons of symmetry only the left-hand side of the density curves is shown.





3.3. Second-order self-energy: expansion formula

According to Eq.(8) we present the imaginary part of the self-energy as a sum of the energy-dependent functions multiplied by \vec{k} -dependent functions (both of them depend on a distance from the central atom). The functions $\in (R^s, \vec{k})$ for successive values of s are as follows:

$$\epsilon(\mathbf{R}^{\circ},\mathbf{k})=1,$$

$$\epsilon (R^{1}, \vec{k}) = 2 [\cos ak_{x} + \cos ak_{y} + \cos ak_{z}],$$

$$\epsilon (R^{2}, \vec{k}) = 2 [\cos a(k_{x} + k_{y}) + \cos a(k_{y} + k_{z}) + \cos a(k_{z} + k_{x}) + \cos a(k_{z} + k_{z}) + \cos a(k_{z} + k_{z})],$$

$$(14)$$

$$= (R^{3}, \vec{k}) = 2 [\cos a (k_{x} + k_{y} + k_{z}) + \cos a (-k_{x} + k_{y} + k_{z}) + \cos a (k_{x} - k_{y} + k_{z}) + \cos a (k_{x} + k_{y} - k_{z})],$$
(16)

$$\in (R^4, \vec{k}) = 2 \left[\cos 2ak_x + \cos 2ak_y + \cos 2ak_z \right], \qquad (17)$$

$$\mathcal{E}(R^{5},\vec{k})=2[\cos a(k_{x}+2k_{y})+\cos a(2k_{x}+k_{y})+\cos a(-k_{x}+2k_{y})++\cos a(2k_{x}-k_{y})+\cos a(k_{x}+2k_{z})+\cos a(2k_{x}+k_{z})++\cos a(-k_{x}+2k_{z})+\cos a(2k_{x}-k_{z})+\cos a(k_{y}+2k_{z})++\cos a(2k_{y}+k_{z})+\cos a(-k_{y}+2k_{z})+\cos a(2k_{y}-k_{z})].(18)$$

In this way, in order to calculate the self-energy at many \vec{k} points of the Brillouin zone, one has to know the functions $S(R^{s}, E)$ (which can be calculated at the beginning of the problem under consideration) and multiply them by functions

(14-18). This procedure is more efficient, even for expansion (8) with a relatively large number of terms than the calculations of the six-dimensional integral (1). In Figs. (3-8) we present the functions $S(R^3, E)$ -see Eq.(8), for s = 0-5. Note, that $S(R^{\circ}, E)$ - Pig. (3), is essentially the local approximation for the imaginary part of the self-energy calculated for U = 1. From the results presented in Figs. (3-8) it is evident that, in principle, the functions $S(R^s, E)$ for greater values of the index S are more oscillating and have smaller absolute values. Nevertheless, in some cases the functions with a greater index 5 can have greater values, compare Figs. (7) and (8), and in addition may be multiplied by $\epsilon(R^{s},\vec{k})$ with greater values than for smaller 5 . In this situation, more distant terms in expansion formula (8) can give larger contributions than other terms. As an example of the use of the expansion formula (8), we present in Fig. (9) the imaginary part of the self-energy calculated for an SCC tight-binding energy band of the bandwidth equal 6 eV. The Fermi energy corresponds to the half-filled energy band and \vec{k} lies in the centre of a Brillouin zone. The dashed curve represents the local approximation (first term in Eq.(8)) and the full line corresponds to Eq.(8) with five terms more included. The small dots located for energies - 3 eV and 3 eV show how the value of the imaginary part of the self-energy changes with increasing number of terms in Eq.(8). One can see that for $\leq =5$ very good convergence is achieved. At other energy points these differences are much smaller. The results of Monte-Carlo integrations are nearly exactly the same for $E > E_F$, even in the neighbourhood of the energy point E = 3 eV (except for variation in the noise). For



Fig. 3. The function $S(R^\circ, E)$ for $\vec{R}^\circ = (000)a$ equivalent with the local approximation for imaginary part of the selfenergy (U = 1.0).



Fig. 4. The function $S(R^{\dagger}, E)$ for \vec{R}^{\dagger} =(100)a.





Fig. 9. The imaginary part of the self-energy for electrons in S-tight-binding energy bands for SCC lattice. The Fermi energy is located at zero energy and bandwidth equals 6 eV. The broken curve is a local approximation and full curve is obtained according Eq.(8). For further explanation - see text.

 $E < E_F$, E = -30 eV the difference exists but is small and equals approximately 5%. We also compared the imaginary part of the self-energy calculated by the Monte-Carlo method and by Eq.(8) for other values of bandfillings and \vec{k} -vectors. For all these cases formula (8) - with six first terms, works very good.

4. Quasiparticle and Kohn-Sham Fermi surfaces

As an example of a practical usage of the results obtained in Sec. 3, we want to check whether the quasiparticle and Kohn-Sham Fermi surfaces coincide with each other. It is well known that the Fermi surface is a well-defined ground-state property of an extended interacting electron system. The quasiparticle Fermi surface may be extracted from the equation

$$\in (\vec{k}) + M(\vec{k},\mu) = \mu$$
 (19)

where $\epsilon(\vec{k})$ are one-electron eigenvalues and $M(\vec{k}, E)$ is a self-energy. The chemical potential μ is U -dependent and can be obtained by fixing the number of electrons. On the other hand, the Kohn-Sham equations in the density functional theory also lead to the Fermi surface /21/. Recently, this problem has been considered by Mearns for an electron gas in a weak external potential /22/ and by Schönhammer and Gunnarsson for electrons on a two-dimensional crystal lattice /23/. In both cases the authors show that. in general, the Kohn-Sham and quasiparticle Fermi surfaces do not coincide. Nevertheless, the case of an electron gas on a three-dimensional lattice was not investigated, mainly because of the enormous numerical effort needed for such investigations. As was shown in Ref. $^{/23/}$, the shape of the Kohn-Sham Fermi surface is U -independent. Therefore, both the Fermi surfaces could be the same when the guasiparticle Fermi surface will be U -independent, too. This will be the case when the second-order self-energy $M(\vec{k}, E)$ evaluated on U =0 Fermi surface will be \vec{k} -independent (for details see $^{23/}$). To check whether the self-energy calculated on a free-electron Fermi surface is \vec{k} -dependent or not, we use formula (8) and take the Fermi surface in a SCC lattice for

S -tight binding energy band corresponding to the bandfilling $N_e = 0.167$ electrons per spin end energy band. For this bandfilling the Fermi surface does not touch the Brillouin zone and for $k_z = 0$ is presented in Fig. (10). Because of the symmetry we show only 1/8 of $k_z = 0$ plane. In the following we calculate the real part of the self-energy along the line depicted in Fig. (10) and the result is shown in Fig. (11) (the imaginary part is identically equal to zero). Here, $\phi = arc \tan(k_x/k_y)$.



Fig. 10. The part of the Fermi surface for U=0. Because of the symmetry, only 1/8 part of the $k_x = 0$ Fermi surface is shown.



Fig. 11. The value of the real part of the self-energy calculated along curve from Fig. (10) for small values of U. The curves A, B and C are calculated using Eq.(8) with 4,5 and 6 terms, respectively. As one can observe, the self-energy calculated on the Fermi surface, Fig. (10), is clearly \vec{k} -dependent. Thus, the quasiparticle and Kohn-Sham Fermi surfaces do not coincide for small in the three dimensional case, too.

5. Conclusions

We have shown that the second-order self-energy for the Hubbard Hamiltonian can be fast calculated in an efficient way according to formula (8) in which the first six terms are included and the \vec{k} -dependence is separated from the E -dependence. Therefore, one can calculate the energy-dependent factors at the beginning and other calculations of the self-energy over the whole Brillouin zone can be immediately performed. The comparison with results obtained within the Monte-Carlo method of integration indicates that for all bandfillings and \vec{k} -vectors formula (8) works very good. As an example of using this algorithm, we have checked whether the quasiparticle Fermi surface in the case of a three-dimensional lattice is equivalent or not to the Kohn-Sham Fermi surface arising in the density-functional theory. Such comparison was made in literature only for a two-dimensional lattice just because of the difficulties in obtaining the self-energy values for a relatively large number of K -vectors. Our investigations performed for three dimensional lattices confirmed earlier results of other authors obtained for other cases.

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