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Moment expansion of the two-particle Green function for the Hubbard Hamiltonian

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Abstract. The energy moment expansion of the two-particle Green function for the Hubbard Hamiltonian is developed by evaluating the corresponding commutators. We calculate explicitly the first four exact moments. These exact results are used to evaluate the accuracy of approximate solutions for the two-particle Green function relevant for the study of the Auger spectra of transition metals.

1. Introduction

The Green function method has been widely used in the study of electron correlations. In particular, it has been employed in the case of the Hubbard Hamiltonian

$$H = \sum_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma} \quad (1)$$

which is broadly used as a model Hamiltonian for strongly correlated electron systems.

The character and the properties of elementary excitations are given by the spectral weight function linearly related to Green function (GF). These functions can be expanded in negative powers of the complex energy z for large $|z|$. The expansion coefficients are called the energy moments. One possible way to evaluate the validity of approximative solutions for GF is to compare the energy moments of the approximate GF with the exact moments. The more energy moments of the approximate GF are correct the more reliable the solution is. The approximate solution usually has only the first few moments correct. It has been suggested [1] that a way of deriving new approximate solutions would be to require that the GF have the correct energy moments.

Let us mention some previous results for the Hubbard Hamiltonian. To our knowledge, the energy moments have been calculated only for the one-particle GF. The situation in this case is as follows. The simplest Hartree–Fock solution gives only the first two moments correctly. The so-called Hubbard I solution [2] is correct in the first three moments. The solution with four correct moments was derived by Tahir-Kheli *et al* [1] with the help of the above mentioned method in the second order.

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In this article we calculate the exact moments for the two-particle GF in order to evaluate the validity of the approximate solutions for this GF which have been used for the explanation of the two-particle spectroscopies (Auger spectra and appearance potential spectra) of transition metals. Several solutions have been developed [3–9], but only some of them [7, 9] are applicable to the case of half-filled band and strong interactions. Recently we have developed a new solution [9] based on the alloy analogy which removes some drawbacks of the simple mean-field solution [7]. The present calculation of the moments was motivated by a need to check further the new solutions.

In section 2 we write the equation of motion for the two-particle GF. In section 3 we develop the exact moment expansion of the two-particle GF. In section 4 the validity of the approximate solutions is discussed.

2. Two-particle Green function

We shall use the double-time Zubarev GF [10] in the same standard notation as in previous papers [7, 9]: i, j, k, l are the site indices, $\sigma = \uparrow, \downarrow$ is the spin index, the momentum indices are k, l, p, q . The retarded two-particle GF in energy representation for complex energy z is

$$G_{ijkl}(z) = \langle\langle a_{i\uparrow} a_{j\downarrow} | a_{i\downarrow}^{\dagger} a_{k\uparrow}^{\dagger} \rangle\rangle_z. \quad (2)$$

In the application to the Auger spectroscopy we are interested in its superdiagonal element $G_o(z) = G_{iiii}(z)$.

The GF $G_{ijkl}(z)$ obeys the equation of motion

$$\begin{aligned} z G_{ijkl}(z) &= \kappa_{ijkl} + \sum_n t_{in} G_{njkl}(z) + \sum_n t_{jn} G_{in kl}(z) \\ &+ U \delta_{ij} G_{ijkl}(z) + U(1 - \delta_{ij}) \Gamma_{ijkl}(z) \end{aligned} \quad (3)$$

where

$$\kappa_{ijkl} = \delta_{ik} \delta_{jl} - \delta_{jl} \langle a_{k\uparrow}^{\dagger} a_{i\uparrow} \rangle - \delta_{ik} \langle a_{i\downarrow}^{\dagger} a_{j\downarrow} \rangle \quad (4)$$

and

$$\Gamma_{ijkl}(z) = \langle\langle (n_{i\downarrow} + n_{j\uparrow}) a_{i\uparrow} a_{j\downarrow} | a_{i\downarrow}^{\dagger} a_{k\uparrow}^{\dagger} \rangle\rangle_z \quad (5)$$

is the higher-order GF. Let us note that equation (3) was obtained by using the derivative of the double-time GF with respect to the left time variable and then transforming to the energy representation.

3. Exact moments

The energy moments m_k entering the expansion of $G_o(z)$

$$G_o(z) = \sum_{k=0}^{\infty} \frac{m_k}{z^{k+1}} \quad (6)$$

are given by

$$m_k = \langle c_{k,m} \rangle \quad c_{k,m} = [A_{k-m}, A_m^{\dagger}] \quad (7)$$

where m is an arbitrary integer $0 \leq m \leq k$. The operators A_m are defined recursively by relations

$$A_0 = a_{0\uparrow} a_{0\downarrow} \quad A_{m+1} = [A_m, H]. \quad (8)$$

Because $\langle c_{k,m} \rangle = \langle c_{k,k-m} \rangle$ and $c_{k,k-m} = c_{k,m}^\dagger$, it holds $\langle c_{n,m} \rangle = \langle c_{n,m}^\dagger \rangle$. Consequently,

$$m_k = \frac{1}{2} \langle c_{k,m} + c_{k,m}^\dagger \rangle. \quad (9)$$

This Hermitian symmetrization allows us to simplify some expressions for higher-order moments and it corresponds to the well known fact that the moments m_k are real numbers.

We have assumed a translationally invariant ground state. In order to simplify the calculations, we have further assumed that the hopping integrals t_{ij} are real and symmetric, $t_{ij} = t_{ji}$, and $t_{ii} = 0$ (centred band). The hopping integrals are connected with the dispersion law of the one-electron band by the relation

$$t_{ij} = \frac{1}{N} \sum_p e^{ip \cdot (R_i - R_j)} E(p). \quad (10)$$

The moments are calculated from the equations (7) and (8) in a straightforward manner. These calculations for higher-order moments are rather cumbersome, so we present here only the first four moments:

$$m_0 = 1 - n \quad (11)$$

$$m_1 = -E_1 + U(1 - n) \quad (12)$$

$$m_2 = (2 - n)W_2 - E_2 - 2UE_1 + U^2(1 - n) \quad (13)$$

$$m_3 = (2 - n)W_3 - E_3 - 3W_2E_1 + 2U(1 + n - p)W_2 - 2UE_2 - 3U^2E_1 + U^3(1 - n) + UC_1 - UC_2 + 2U^2C_3 \quad (14)$$

where $n = \sum_\sigma \langle a_{i\sigma}^\dagger a_{i\sigma} \rangle$ is the concentration of electrons, $p = \langle n_{i\uparrow} n_{i\downarrow} \rangle$, and

$$W_k = \frac{1}{N} \sum_q E_q^k \quad E_k = \frac{1}{N} \sum_q \sum_\sigma n_{q\sigma} E_q^k. \quad (15)$$

Here

$$n_{q\sigma} = \sum_i e^{-iq \cdot (R_i - R_j)} \langle a_{i\sigma}^\dagger a_{j\sigma} \rangle \quad (16)$$

is the occupation number of the Bloch state with the wave vector q . The correlation functions C_1 , C_2 and C_3 are defined as

$$C_1 = \frac{1}{N^2} \sum_{kpq\sigma} \{ \frac{1}{4} [E(q) + E(k - q) - E(p) - E(k - p)]^2 - \frac{1}{2} [E(q) - E(k - p)] [E(p) - E(k - q)] \} + \frac{1}{N} \sum_l E(l - k) E(l - p - q) \langle a_{k-p\sigma}^\dagger a_{k-q\sigma} a_{p\sigma}^\dagger a_{q\sigma} \rangle \quad (17)$$

$$C_2 = \frac{1}{N^2} \sum_{kpq\sigma} [\frac{1}{2} E(p - q) E(p) + \frac{1}{2} E(k + q) E(k) + \frac{1}{N} \sum_l E(q - l) E(l)] \langle a_{k\sigma}^\dagger a_{p\sigma}^\dagger a_{p-q\sigma} a_{k+q\sigma} \rangle \quad (18)$$

$$C_3 = \frac{1}{N} \sum_k E(k) S(k) \quad S(k) = \frac{1}{N} \sum_{ij\sigma} e^{ik \cdot (R_i - R_j)} \langle n_{i\sigma} n_{j\sigma} a_{i\sigma}^\dagger a_{j\sigma} \rangle. \quad (19)$$

4. Comparison of approximate solutions

Recently we have developed two approximate solutions of the hierarchy of equations for the GF G_{ijkl} . Both use the decoupling for the GF Γ in equation (3). The first, Hartree-Fock-like solution [7], is based on the approximation

$$\Gamma_{ijkl}(z) \approx (n_{i\downarrow} + n_{j\uparrow})G_{ijkl}(z). \quad (20)$$

This solution is applicable to any electron concentration $0 \leq n \leq 2$ and to any interaction strength U , has the correct behaviour with respect to the electron-hole transformation and is correct in four exactly solvable limiting cases [7]. However, it is not a genuine interpolating solution between the weak and strong interaction regimes because it is not correct in the neighbourhood of the atomic limit.

The second solution [9] improves the previous one in the regime of the strong interactions. It was derived using the more complicated alloy analogy decoupling

$$\Gamma_{ijkl} \approx \epsilon_{ij} G_{ijkl} \quad (21)$$

where ϵ_{ij} is a random variable taking three values corresponding to the situations in which none, one or two electrons, respectively, occupy the states at sites i and j . In this way we have replaced the electron correlation problem by the problem of the disordered ternary inhomogeneous alloy which is treated within the coherent potential approximation (CPA). We also make a comparison with the approximate theory derived by Presilla and Sacchetti [6]. This solution also has the correct band and atomic limit (in the case of the single band); however, it violates the electron-hole symmetry.

The explicit expression for the superdiagonal element $G_o(z)$ of the two-particle GF within these three approximations can be summarized as follows.

$$G_o(z) = \frac{1}{N^2} \sum_{kq} \frac{1}{1 - V(z)\Psi_o(k, \xi)} \frac{1 - n_{k-q\uparrow} - n_{q\downarrow}}{\xi - E(k - q) - E(q)} \quad (22)$$

where ξ is the renormalized energy and $V(z)$ is the renormalized strength of the pair interaction. The choice

$$V = U \quad \xi = z \quad (23)$$

yields the result of Presilla and Sacchetti [6], while

$$V = U(1 - n) \quad \xi = z - Un \quad (24)$$

gives the Hartree-Fock-like solution [7]. Finally, the choice

$$V = U - \Sigma(z) \quad \xi = z - \Sigma(z) \quad (25)$$

corresponds to the alloy analogy solution [9]. Here $\Sigma(z)$ is the self-energy obtained by solving the CPA equation

$$\sum_{k=0}^2 c_k \frac{Uk - \Sigma(z)}{1 - (Uk - \Sigma(z))F(z)} = 0 \quad (26)$$

where

$$F(z) = \frac{1}{N^2} \sum_{kq} \frac{1}{z - \Sigma(z) - E(k - q) - E(q)} \quad (27)$$

and c_k are the concentrations entering the effective alloy problem (for details see [9]). The moments are found from the expansion of (22) in negative powers of z for large $|z|$.

The four lowest moments for these approximative solutions are (the superscripts PS, HF, and CPA are self-explanatory)

$$m_0^{\text{PS}} = m_0^{\text{HF}} = m_0^{\text{CPA}} = m_0 \quad (28)$$

$$m_1^{\text{PS}} = m_1^{\text{HF}} = m_1^{\text{CPA}} = m_1 \quad (29)$$

$$m_2^{\text{PS}} = m_2 + U E_1 \quad (30)$$

$$m_2^{\text{HF}} = m_2^{\text{CPA}} = m_2 + U(1-n)E_1 \quad (31)$$

$$m_3^{\text{PS}} = \mu_3 + U[(4-3n)W_2 - E_2] - U^2 E_1 \quad (32)$$

$$m_3^{\text{HF}} = \mu_3 + U(4-n-n^2)W_2 - U(1+2n)E_2 - U^2(1+n+n^2)E_1 \quad (33)$$

$$m_3^{\text{CPA}} = \mu_3 + U(4-n-n^2)W_2 - U(1+2n)E_2 - U^2(1+2n+2p)E_1. \quad (34)$$

The quantity μ_3 is a shorthand for the expression

$$\mu_3 = (2-n)W_3 - E_3 - 3W_2 E_1 + U^3(1-n). \quad (35)$$

Hence, all three solutions reproduce only the first two moments exactly. The Hartree-Fock-like and the alloy analogy theory yield the same (incorrect) value of the third moment. Let us note that it becomes exact for the half-filled band, or for the empty band ($E_1 = 0$). These two solutions start to have different moments from the fourth one. In this case the moment for the alloy analogy solution contains the two-particle correlation function p , which is completely absent in the Hartree-Fock-like solution (and also in the solution of Presilla and Sacchetti). It corresponds to an improvement of the former solution over the latter in the strong-correlation regime. However, the correlation function p appears in different terms than in the exact solution. Moreover, the two- and three-site correlation functions are not contained in fourth and higher moments for either approximate solution. The third moment of Presilla and Sacchetti's solution is correct only in the case of the empty band ($E_1 = 0$).

5. Conclusion

We presented the method of the calculation of the energy moments of the two-particle GF for the Hubbard Hamiltonian. We used these exact results to evaluate the validity of three approximate solutions obtained by decoupling in the equations of motion for the two-particle GF. The corresponding moments differ from the exact ones already in the third order. In order to get the solution with the correct third moment one could try to follow the method suggested by Tahir-Kheli [1]. It can be described as follows. The hierarchy of the equations of motion is terminated at the n th level approximating the GF of the $(n+1)$ th order by a linear combination of the GFs of the lower order. The coefficients of this combination are determined from the condition that GF of the n th order obtained by this decoupling have the correct first n non-trivial moments. The work in this direction is in progress.

The criterion of the number of correct moments is only very rough and a more quantitative analysis is desirable. However, it is complicated by the absence of the exact results for many-particle correlation functions which enter the higher-order moments. Another possibility for getting more information is to analyse the moments for individual peaks in the spectral weight function instead of the full moments in a way similar to the analysis by Harris and Lange [11] in the case of the one-particle GF for the original Hubbard solutions.

Acknowledgments

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References

- [1] Tahir-Kheli R A and Jarrett H S 1969 *Phys. Rev.* **180** 544
- [2] Hubbard J 1963 *Proc. R. Soc. A* **276** 238
- [3] Cini M 1979 *Surf. Sci.* **87** 483
- [4] Drchal V and Kudrnovský J 1984 *J. Phys. F: Met. Phys.* **14** 2443
- [5] Treglia G, Desjonqueres M C, Ducastelle F and Spanjaard D 1981 *J. Phys. C: Solid State Phys.* **14** 4377
- [6] Presilla C and Sacchetti F 1987 *J. Phys. F: Met. Phys.* **17** 779
- [7] Drchal V 1989 *J. Phys.: Condens. Matter* **1** 4773
- [8] Kotrla M and Drchal V 1989 *J. Phys.: Condens. Matter* **1** 4783
- [9] Kotrla M and Drchal V 1992 *J. Phys.: Condens. Matter* **4** 4251
- [10] Zubarev D N 1960 *Sov. Phys.-Usp.* **3** 320
- [11] Harris A B and Lange R V 1967 *Phys. Rev.* **157** 295