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The Mott transition in the strong coupling perturbation theory

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ABSTRACT

Using the strong coupling diagram technique a self-consistent equation for the electron Green's function is derived for the repulsive Hubbard model. Terms of two lowest orders of the ratio of the bandwidth Δ to the Hubbard repulsion U are taken into account in the irreducible part of the Larkin equation. The obtained equation is shown to retain causality and reduces to Green's function of uncorrelated electrons in the limit $U\to 0$. Calculations were performed for the semi-elliptical initial band. It is shown that the approximation describes the Mott transition, which occurs at $U_c=\sqrt{3}\Delta/2$. This value coincides with that obtained in the Hubbard-III approximation. At half-filling, for $0<U<U_c$ the imaginary part of the self-energy is nonzero at the Fermi level, which indicates that the obtained solution is not a Fermi liquid. At small deviations from half-filling the density of states shifts along the frequency axis without perceptible changes in its shape. For larger deviations the density of states is modified: it is redistributed in favor of the subband, in which the Fermi level is located, and for $U>U_c$ the Mott gap disappears.

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1. Introduction

The repulsive Hubbard model is one of the main models describing strong electron correlations in crystals. For its investigation a number of methods is used, discussion of which can be found, in particular, in reviews [1–4]. This paper is devoted to the development of one of such methods – the strong coupling diagram technique. As follows from its name, the method is aimed at the limit of strong Hubbard repulsion U, when it is comparable or larger than the width of the initial electron band Δ. However, due to peculiarities of the method it gives the correct result also in the limit $U\to 0$ thereby providing an interpolation between the two limits. In calculating Green's functions the method uses the serial expansion in powers of hopping constants. The elements of the arising diagram technique are site cumulants of different orders, connected by hopping lines. As in the diagram technique with the expansion in powers of an interaction, in the present approach the linked-cluster theorem allows one to discard disconnected diagrams and to carry out partial summations in connected diagrams. As a result the one-particle Green's function is expressed in the form of the Larkin equation through the initial electron dispersion and the sum of all irreducible diagrams – the diagrams, which cannot be divided into two disconnected parts by cutting some hopping line. For more details see Refs. [5–9]. A somewhat different diagram technique, which is also based on the serial expansion in powers of hopping constants, was developed in Refs. [10–13]. Elements of this latter technique are Green's functions of Hubbard operators and end parts. In principle, both diagram techniques give identical results if consistent diagrams are chosen. However, the diagram technique for Hubbard operators is less convenient, since the system of operator pairings is not unique, being dependent on the chosen precedence of operators, and the number of diagrams is much larger in comparison with the technique based on cumulants.

In this paper we consider one-site contributions of the first two orders to the mentioned sum of irreducible diagrams. With the insertion of the first- and second-order diagrams into internal hopping lines, the used approximation gives an equation for self-consistent determination of the electron Green's function. It is shown that the solution of this equation retains causality. For small U the equation reduces to the Hartree solution, and for $U=0$ it gives Green's function of uncorrelated electrons. Hence the obtained equation provides an interpolation between cases of the week and strong coupling. Calculations were carried out for a semi-elliptical initial band. The approximation is able to describe the Mott transition, which takes place at $U_c=\sqrt{3}\Delta/2$. This value coincides with that found in the Hubbard-III approximation [14]. However, in contrast to this latter approximation the obtained density of states (DOS) reduces to the initial semi-elliptical DOS at $U=0$. At half-filling, for $0<U<U_c$ the imaginary part of the self-energy is nonzero at the Fermi level, while it is small for $U\ll U_c$. Hence the obtained solution does not correspond to the Fermi liquid. At half-filling the self-energy at the Fermi level diverges as $U\to U_c$ from either of sides. No quasiparticle peak, inherent in the dynamic mean field approximation, is observed in our calculations

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at the Mott transition. At small deviations from half-filling the DOS shifts along the frequency axis without perceptible change in its shape. For larger deviations the DOS is redistributed in favor of the subband, in which the Fermi level is located, and for $U > U_c$ the Mott gap disappears. Possible ways of the inclusion of spin and charge fluctuations into the theory are briefly discussed.

2. Main formulas

We shall consider the repulsive Hubbard model on a two-dimensional (2D) square lattice. The model is described by the Hamiltonian

$$H = \sum_{\mathbf{nn}'\sigma} t_{\mathbf{nn}'} a^{\dagger}_{\mathbf{n}\sigma} a_{\mathbf{n}'\sigma} + \frac{U}{2}\sum_{\mathbf{n}\sigma} n_{\mathbf{n}\sigma} n_{\mathbf{n},-\sigma}, \tag{1}$$

where $t_{\mathbf{nn}'}$ is the hopping constants, the operator $a^{\dagger}_{\mathbf{n}\sigma}$ creates an electron on the site $\mathbf{n}$ of the 2D lattice with the spin projection $\sigma = \pm 1$ and the electron number operator $n_{\mathbf{n}\sigma} = a^{\dagger}_{\mathbf{n}\sigma} a_{\mathbf{n}\sigma}$. In this work we shall calculate the electron Green's function

$$G(\mathbf{n}'\boldsymbol{\tau}', \mathbf{l}\boldsymbol{\tau}) = \langle \mathcal{T}\, \overline{a}_{\mathbf{n}'\sigma}(\tau') a_{\mathbf{n}\sigma}(\tau)\rangle, \tag{2}$$

where the angular brackets denote the statistical averaging with the Hamiltonian $\mathcal{H} = H - \mu\sum_{\mathbf{n}\sigma} n_{\mathbf{n}\sigma}$, μ is the chemical potential, $\mathcal{T}$ is the time-ordering operator which arranges operators from right to left in ascending order of times τ, $a_{\mathbf{n}\sigma}(\tau) = \exp(\mathcal{H}\tau) a_{\mathbf{n}\sigma} \exp(-\mathcal{H}\tau)$ and $\overline{a}_{\mathbf{n}\sigma}(\tau) = \exp(\mathcal{H}\tau) a^{\dagger}_{\mathbf{n}\sigma} \exp(-\mathcal{H}\tau)$. Green's function (2) does not depend on the spin projection, and it was omitted in the function notation.

In the strong coupling diagram technique Green's function (2) is presented as the serial expansion in powers of the kinetic term in the Hamiltonian, and the role of the unperturbed Hamiltonian is played by the repulsion term of Eq. (1) together with the term containing the chemical potential

$$\mathcal{H}_0 = \sum_{\mathbf{n}} \mathcal{H}_{\mathbf{n}},$$
$$\mathcal{H}_{\mathbf{n}} = \sum_{\sigma}\left(\frac{U}{2} n_{\mathbf{n}\sigma} n_{\mathbf{n},-\sigma} - \mu n_{\mathbf{n}\sigma}\right). \tag{3}$$

Terms of the series are constructed from the hopping constants $t_{\mathbf{nn}'}$ and cumulants of the operators $a_{\mathbf{n}\sigma}(\tau)$ and $\overline{a}_{\mathbf{n}\sigma}(\tau)$ belonging to the same site. The cumulants are calculated with the site Hamiltonian $\mathcal{H}_{\mathbf{n}}$, Eq. (3). The sum of all terms of the series can be written in the form of the Larkin equation

$$G(\mathbf{k}, i\omega_l) = \frac{K(\mathbf{k}, i\omega_l)}{1 - t_{\mathbf{k}} K(\mathbf{k}, i\omega_l)}, \tag{4}$$

where the Fourier transformation over the space and time variables was performed, $\mathbf{k}$ is the 2D wave vector, $\omega_l = (2l+1)\pi T$ is the Matsubara frequency with the temperature T, $t_{\mathbf{k}} = \sum_{\mathbf{n}} \exp[i\mathbf{k}(\mathbf{n} - \mathbf{n}')] t_{\mathbf{nn}'}$ and $K(\mathbf{k}, i\omega_l)$ is the sum of all irreducible diagrams, which is termed the irreducible part of the Larkin equation. Terms of lowest orders in this sum are shown in Fig. 1 together with their signs and prefactors. Here circles denote cumulants, which orders equal to numbers of incoming or outgoing directed lines. Two outer arrows designate the operators $\overline{a}_{\mathbf{n}'\sigma}(\tau')$ and $a_{\mathbf{n}\sigma}(\tau)$ of Green's function (2) in cumulants. The discussed diagram technique allows a partial summation. Therefore, it is presumed that irreducible diagrams of all orders and in all possible combinations are inserted in the internal hopping lines – the arrowed lines in the diagrams in Fig. 1. As a result, in the diagrams, the bare hopping $t_{\mathbf{k}}$ is substituted by the renormalized one

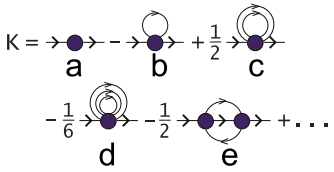

Fig. 1. Irreducible diagrams of the first four orders in the irreducible part $K(\mathbf{k}, i\omega_l)$.

$$\theta(\mathbf{k}, i\omega_l) = \frac{t_{\mathbf{k}}}{1 - t_{\mathbf{k}} K(\mathbf{k}, i\omega_l)} = t_{\mathbf{k}} + t^2_{\mathbf{k}} G(\mathbf{k}, i\omega_l). \tag{5}$$

The sign of a term in the irreducible part $K(\mathbf{k}, i\omega_l)$ is equal to $(-1)^L$, where L is the number of loops formed by hopping lines. Prefactors in the diagrams arise due to the fact that some permutations of the kinetic energy Hamiltonians in a power expansion term lead to the same diagram, since creation and annihilation operators of these permuted Hamiltonians enter into the same cumulant. At any cumulant the conservation laws of the number of particles, energy and momentum are maintained.

Notice that this approach can be used also for calculating many-particle Green's functions. In Ref. [9] dynamic spin and charge susceptibilities of the one-band repulsive Hubbard model were investigated by summing infinite sequences of ladder diagrams. The approach reproduces correctly a number of magnetic properties inherent in the strong-coupling limit, in particular, the establishment of the long-range antiferromagnetic order when the temperature is lowered and the Curie law for the susceptibility.

The first-order cumulant coincides with the one-particle site Green's function. A cumulant of an order $\nu > 1$ is equal to the ν-particle site Green's function and a sum of all possible products of lower-order cumulants, the summarized orders of which are equal to ν. The sign, with which a term appears in this sum, is equal to $-(-1)^P$, where P is the number of permutations performed to obtain the order of operators in the term from that in the νth cumulant. In other words, the signs of the terms containing products of first-order cumulants are opposite to signs of the same terms, which would arise from the ν-particle Green's function in the νth cumulant if Wick's theorem [15] were applicable. As a result in the limit $U \to 0$ all cumulants of orders $\nu > 1$ vanish, and with them all irreducible diagrams in $K(\mathbf{k}, i\omega_l)$ become equal to zero, except the diagram (a) in Fig. 1. The first-order cumulant in this latter diagram reads

$$C_1(i\omega_l) = -\int_0^{\beta} d\tau e^{i\omega_l \tau} \langle a_{\mathbf{n}\sigma}(\tau) \overline{a}_{\mathbf{n}\sigma}\rangle$$
$$= \frac{1}{Z}[(e^{-\beta E_1} + e^{-\beta E_0}) g_{01}(i\omega_l) + (e^{-\beta E_2} + e^{-\beta E_1}) g_{12}(i\omega_l)], \tag{6}$$

where $\beta = 1/T$, $E_0 = 0$, $E_1 = -\mu$ and $E_2 = U - 2\mu$ are eigenvalues of the site Hamiltonian $H_{\mathbf{n}}$, Eq. (3), the partition function $Z = e^{-\beta E_0} + 2e^{-\beta E_1} + e^{-\beta E_2}$, $g_{ij}(i\omega_l) = (i\omega_l + E_i - E_j)^{-1}$, i and $j = 0, 1$ and 2. Substituting $(i\omega_l + \mu)^{-1}$, the value of $C_1(i\omega_l)$ at $U = 0$, into Eq. (4) we obtain the correct expression for Green's function of uncorrelated electrons. Thus, the considered approach has an important property – despite the fact that Eq. (4) was derived from the expansion in powers of $t_{\mathbf{nn}'}/U$, it gives the correct result in the limit $U \to 0$.

In the following consideration we take into account only the one-site diagrams (a) and (b) in Fig. 1. Thus, in Eq. (4) the irreducible part does not depend on the wave vector and is given by the equation

$$K(i\omega_l) = C_1(i\omega_l)$$
$$-\frac{T}{N}\sum_{\mathbf{k}l'\sigma'} C_2(i\omega_l, \sigma; i\omega_l, \sigma; i\omega_{l'}, \sigma'; i\omega_{l'}, \sigma')$$
$$\times \theta(\mathbf{k}, i\omega_{l'}), \tag{7}$$

where N is the number of lattice sites and C_2 is the Fourier transform of the second-order cumulant

$$C_2(\tau_1\sigma, \tau_2\sigma, \tau_3\sigma', \tau_4\sigma')$$
$$= \langle \mathcal{T}\, \overline{a}_{\mathbf{n}\sigma}(\tau_1) a_{\mathbf{n}\sigma}(\tau_2) \overline{a}_{\mathbf{n}\sigma'}(\tau_3) a_{\mathbf{n}\sigma'}(\tau_4)\rangle$$
$$- \langle \mathcal{T}\, \overline{a}_{\mathbf{n}\sigma}(\tau_1) a_{\mathbf{n}\sigma}(\tau_2)\rangle \langle \mathcal{T}\, \overline{a}_{\mathbf{n}\sigma'}(\tau_3) a_{\mathbf{n}\sigma'}(\tau_4)\rangle$$
$$+ \langle \mathcal{T}\, \overline{a}_{\mathbf{n}\sigma}(\tau_1) a_{\mathbf{n}\sigma'}(\tau_4)\rangle \langle \mathcal{T}\, \overline{a}_{\mathbf{n}\sigma'}(\tau_3) a_{\mathbf{n}\sigma}(\tau_2)\rangle.$$

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