Ground State of Strongly Correlated Fermions: Short-Range Order

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A new variational method is developed to calculate the ground state energy of Fermi systems with strong short-range correlations. A trial wave function of Gutzwiller’s type contains additional variational parameters corresponding to configurations of pairs of nearest-neighbor sites. To evaluate the ground state energy, generalized Kikuchi’s pseudo-ensemble method is used. The Hubbard model at half band-filling is investigated. The ground state energy of the paramagnetic phase is calculated for a chain, square and simple cubic lattices. It is shown that the short-range order lowers drastically the ground state energy of the Hubbard model at intermediate interaction strength. The paramagnetic phase of the Kondo-Hubbard model (\(S = 1/2\) and \(S = 5/2\)) at half band-filling is investigated. The ground state energy, correlation functions and effective mass are calculated for chain, square and simple cubic lattices. A phase transition was found for simple cubic lattice.

71.10.Fd, 71.10.Hf, 71.27.+a, 71.28.+d

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I. INTRODUCTION

A short-range order, i.e., strong short-range correlations, is an intrinsic feature of strongly correlated Fermi systems. It was observed in a metal phase of V$_2$O$_3$ - a famous Mott-Hubbard system [2], high-temperature superconductors [2], and heavy fermion systems [2-3]. Principal aspects of the short-range order can be investigated within the Hubbard model [2]. The exact solution of the Hubbard Hamiltonian is known for 1D chain [10]. Great simplifications appear in infinite dimensions, which are of great practical importance, one has to follow various numerical and analytical approximations [2-4]. Recently a new variational approach to the ground state of the Hubbard model was proposed [12,14]. In addition to intrasite correlations the trial wave function of Gutzwiller’s type [3] contains nearest-neighbor correlations in an explicit form. In contrast to Ref. [14], Kikuchi’s (cluster variation) method [15] was used to evaluate the ground state energy. It was shown that the short-range correlations affect significantly the ground state of the Hubbard model. A comparison of this result with the variational Monte Carlo method (VMC) [16] based on the Gutzwiller trial wave function and $1/D$-expansion in the dynamical mean-field theory [18] shows that the latters underestimate significantly the ground state energy at intermediate coupling.

A heavy fermion behavior usually arises from an interplay between a lattice of localized $f$-electrons and itinerant electrons. In the Kondo limit, such a system becomes a Kondo lattice [19]. In many cases the itinerant subsystem of the Kondo lattice is formed by a narrow $d$-band where the short-range Coulomb interaction between itinerant electrons is considerable. There is a lot of examples of this kind [13]. Therefore it is reasonable to describe the itinerant subsystem by means of the Hubbard Hamiltonian. Thus, we come to the Kondo-Hubbard lattice model [20]. It was shown by means of neutron scattering experiments that strong short-range antiferromagnetic (AFM) correlations exist in Kondo and Kondo-Hubbard lattices [3-4]. They play an important role in the heavy fermion behavior. In this paper, I apply the variational theory of Ref. [14] to the Kondo-Hubbard lattice model. In Sec.II, the variational technique is introduced. The ground state energy of the paramagnetic (PM) phase of the Hubbard model at half-band filling is calculated. In Sec.III, the technique is generalized to the Kondo-Hubbard lattice model. The ground state energy, correlation functions, and effective mass are calculated at half-band filling for (i) spin $1/2$ and (ii) spin $5/2$ ($f$-spin) Kondo-Hubbard lattices. The results are discussed in Sec.IV.

II. GROUND STATE OF THE HUBBARD MODEL

A. Trial Wave Function

Let us consider a lattice with one orbital per site and restrict ourselves to nearest-neighbor hopping only. Then, the Hubbard model has the following form

$$H_{H} = t \sum_{\langle ij \rangle, \sigma} \left( a_{i\sigma}^\dagger a_{j\sigma} + \text{H.c.} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

where $a_{i\sigma}^\dagger (a_{i\sigma})$ is the creation (annihilation) operator of a fermion of spin $\sigma = \uparrow, \downarrow$ on the $i$-th lattice site, $\langle ij \rangle$ denotes a pair of adjacent sites, $n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma}$.

The Gutzwiller trial wave function [3] gives a good basis for a variational analysis of the Hubbard model ground state in infinite dimensions. This trial function can be written in the following symbolic form [21]

$$|\psi\rangle = g_0 \hat{X} |\varphi_0\rangle$$

where $\hat{X} = \sum_i n_{i\uparrow} n_{i\downarrow}$, $g_0$ is the real parameter taking a value in the interval $[0, 1]$ if $U \geq 0$, $|\varphi_0\rangle$ is the $N$-particle wave function of non-interacting fermions, for instance

$$|\varphi_0\rangle = \prod_{k \in V_F^\uparrow} a_{k\uparrow}^\dagger \prod_{k \in V_F^\downarrow} a_{k\downarrow}^\dagger |0\rangle.$$ 

Here, $a_{k\sigma}^\dagger$ denotes the creation operator of the Bloch state, $k$ is the wave vector, and $V_{F\sigma}$ is the space within the Fermi surface.

To control nearest-neighbor correlations between fermions one can extend the Gutzwiller trial wave function as [10]

$$|\psi\rangle = \prod_{\lambda} g_{\lambda} \hat{P}_{\lambda} |\varphi_0\rangle$$

where $\hat{P}_{\lambda}$ are the projection operators onto all feasible configurations of a single site and a pair of nearest-neighbor sites, $g_{\lambda}$ are the nonnegative real parameters. In the PM phase, there are 4 such operators for intrasite configurations

$$\hat{X}_1 = \sum_i (1 - n_{i\uparrow}) (1 - n_{i\downarrow}),$$
$$\hat{X}_2 = \sum_i n_{i\uparrow} (1 - n_{i\downarrow}),$$
$$\hat{X}_3 = \sum_i (1 - n_{i\uparrow}) n_{i\downarrow},$$
$$\hat{X}_4 = \sum_i n_{i\uparrow} n_{i\downarrow},$$

and 10 operators for nearest-neighbor configurations.
\[ \hat{Y}_1 = \sum_{(ij)} (1 - n_i^\uparrow) (1 - n_i^\downarrow) (1 - n_j^\uparrow) (1 - n_j^\downarrow), \]

\[ \hat{Y}_2 = \sum_{(ij)} n_i^\uparrow n_i^\downarrow n_j^\uparrow n_j^\downarrow, \text{ and etc.} \]

All the operator \( \hat{Y}_\lambda \) and corresponding pair configurations are shown in Table II.

From now on, we shall consider only lattices for which the total number of nearest-neighbors pairs is equal to \( zL/2 \), where \( z \) is the number of the nearest neighbors of a site and \( L \) is the total number of sites. Let us denote normalized eigenvalues of the projection operators as \( x_\lambda |\Phi\rangle = L^{-1} \hat{X}_\lambda |\Phi\rangle, y_\lambda |\Phi\rangle = (zL/2)^{-1} \hat{Y}_\lambda |\Phi\rangle \). The eigenvalues turn out to be related to each other by normalization conditions \[ \sum_\lambda x_\lambda = 1, \quad \sum_\lambda \beta_\lambda y_\lambda = 1 \] and self-consistency conditions \[ y_1 + y_3 + y_4 + y_5 = x_1, \]
\[ y_2 + y_3 + y_8 + y_9 = x_4, \]
\[ y_4 + y_6 + y_7 + y_8 = x_2, \]
\[ y_5 + y_7 + y_9 + y_{10} = x_3. \]

As concentrations of fermions of each spins are fixed there are the only independent parameter \( x_\lambda \) and 7 independent parameters \( y_\lambda \). In the case of half band-filling, additional constrains appear
\[ y_1 = y_2, \quad y_6 = y_{10}, \quad y_4 = y_5 = y_8 = y_9 \]
which reduce the number of the independent parameters \( y_\lambda \) to 3. Assume that \( x_1 = x_4 = x, y_3, y_4, \) and \( y_7 \) are the independent parameters. Then, we obtain the final form of the generalized trial wave function of the PM phase at half band-filling
\[ |\psi\rangle = g_0^X g_3^Y g_4^4 g_7^g \hat{Y}_3 \hat{Y}_4 \hat{Y}_7 |\varphi_0\rangle. \]

To elucidate the physical meaning of the trial function \[ \text{(3)} \] let us rewrite the initial wave function of non-interacting fermions as a superposition of configurations
\[ |\varphi_0\rangle = \sum_\Gamma A_\Gamma |\Gamma\rangle, \]
\[ |\Gamma\rangle = \prod_i \alpha_{i\sigma}^\dagger |0\rangle \]
where \( A_\Gamma \) is the complex amplitude of the configuration \( \Gamma \), \( |0\rangle \) is the vacuum state. Then, we obtain
\[ |\psi\rangle = \sum_\Gamma g_0^{D_{\Gamma}} g_3^{2D_{\Gamma3}} g_4^{gD_{\Gamma4}} g_7^{2D_{\Gamma7}} A_\Gamma |\Gamma\rangle \]
Here \( D_{\Gamma0} \) denotes the number of doubly occupied sites in the configuration \( \Gamma \), \( D_{\Gamma3(4,7)} \) are the numbers of configurations of nearest-neighbor pairs corresponding to the operator \( \hat{Y}_3, \hat{Y}_4, \) and \( \hat{Y}_7 \) in the configuration \( \Gamma \). Since other operators \( \hat{Y}_\lambda \) are related to them by Eqs.\[ \text{(3)}, \text{(4)}, \text{and (6)}, \] all the possible configurations of nearest-neighbor pairs are taken into account explicitly.

Since the operator \( \hat{F} = g_0^X g_3^{\beta_3 \hat{Y}_3} g_4^{4 \beta_4 \hat{Y}_4} g_7^g \beta_7 \hat{Y}_7 \) is a polynomial of \( n_{i\sigma} \), it commutes with an operator of particle alternation. Thus, the trial wave function \[ \text{(3)} \] is antisymmetric. \( \hat{F} \) is also invariant under the operations transforming lattice into itself, namely, translations, reflections, rotations and inversion. This means that all the symmetries of the initial wave function remain valid for the trial wave function.

**B. Ground State Energy of the PM phase**

It is well known that correlations between fermions of the same spin exist even in the initial state \[ \text{(3)}, \] i.e. at \( U = 0 \). That is why, first we should evaluate its norm using an equiprobable state. The norm of a correlated state is calculated also using the equiprobable state. Finally, all expressions should be normalized to the norm of the initial state \[ \text{(3)}. \]

Since operators \( \hat{F} \) make up an operator group \( \{ \hat{F}(g_0, g_3, g_4, g_7) \} \)\( \hat{F}(g_0, g_3, g_4, g_7) = \hat{F}(g_0 g_0, g_3 g_3, g_4 g_4, g_7 g_7) \) and \( \hat{F}^{-1} = 1 \) when \( g_\lambda \) are finite and nonzero) this procedure is equivalent to applying the Fermi sea state \[ \text{(3)} \] as the initial one in Eq.\[ \text{(5)}. \]
Thus, the norm of any state generated by Eq.\[ \text{(5)}. \] is \[ \text{(6)}. \]

\[ \langle \psi | \psi \rangle = \sum_\{x, y_3, y_4, y_7\} W(x, y_3, y_4, y_7, g_{\lambda})^2 L_{x} L_{y_3} L_{y_4} L_{y_7}, \]
\[ = \sum_\{x, y_3, y_4, y_7\} R(x, y_3, y_4, y_7). \]

A factor which is inessential for the further calculations is dropped in Eq.\[ \text{(10)}. \] The summation is performed over all the sets \( \{x, y_3, y_4, y_7\} \). A lot of configurations are related to the same set of the independent variables. Then, \( W(x, y_3, y_4, y_7) \) is the number of the configurations corresponding to the fixed set \( \{x, y_3, y_4, y_7\} \) or the weight of this set. To calculate this quantity we use Kikuchi’s pseudo-ensemble method \[ \text{(7)}. \]

It should be mentioned that this method is practically exact for Bethe lattices and approximate for lattices with closed paths \[ \text{(22)}. \] According to Kikuchi’s hypothesis the weight of a set can be expressed as a product \[ \text{(8)}. \]

\[ W = \Gamma Q \]

Here, lower indices are omitted for the sake of simplicity. The quantity \( Q \) determines the number of arrangements of ten indistinguishable elements corresponding to \( \hat{Y}_\lambda \) at \( zL/2 \) pairs, i.e. the multinomial coefficients

\[ Q = \frac{10!}{\prod_\lambda \left( \frac{5 + 5}{2} \right)!} \beta_\lambda, \]

and
\[
\Gamma = \frac{L! \prod \lambda (x\lambda z L)!}{(z L)! \prod \lambda (x\lambda L)!}
\]  
\tag{13}
\]
is the fraction of proper arrangements in the pseudo-ensemble \[24\]. In Eqs.\(12\) and \(13\) the dependent variables should be expressed in terms of \(x, y_3, y_4, y_7\) as follows
\[
x_2 = x_4 = 1/2 - x,
\]
\[
y_1 = y_2 = x - y_3 - 2y_4,
\]
\[
y_6 = y_{10} = 1/2 - x - y_7 - 2y_4.
\]  
\tag{14}

From now on, we use \(y_2\) and \(y_6\) as brief notations of the expressions \(\[14\]\).

In the thermodynamic limit \((L \to \infty)\) we can retain, in the usual fashion \[15\],\[24\], only the terms of the series \(\[10\]\) which are very close to the largest one that is the following condition should be valid \((x, y_3, y_4, y_7) \to (x, y_3, y_4, y_7)_{M A X}\). All the other terms are exponentially small. Since \(R\) is a nonnegative function, it is convenient to search the global maximum of its logarithm rather than of itself. Let us transform the factorials involved in \(R\) by means of the asymptotic Stirling formula. Then, let us find the logarithm of \(R\) and retain the leading term on \(L\) only. A straightforward calculation yields
\[
L^{-1} \ln W = 2(z-1) [x \ln x + (1/2 - x) \ln (1/2 - x)]
\]
\[
- z(y_2 \ln y_2 + y_3 \ln y_3 + 4y_4 \ln y_4
\]
\[
+ y_6 \ln y_6 + y_7 \ln y_7).
\]  
\tag{15}

The domain of function \(\[13\]\) is limited by conditions \(\[3\]\) and \(\[3\]\). It can be shown that the gradient of the function at boundaries is directed inwards to the domain. Therefore the global maximum of \(R\) is an internal one and conditions
\[
\frac{\partial (\ln R)}{\partial x} = 0,
\]  
\tag{16}

where \(\eta_i = x, y_3, y_4, y_7\), are necessary for the global maximum. They lead to the following system of equations that relate \(g_i\) to \(x\) and \(y_i\):
\[
g_0 = \left(\frac{1/2 - x}{x}\right)^{z-1} \left(\frac{x - y_3 - 2y_4}{1/2 - x - y_7 - 2y_4}\right)^{z/2},
\]
\[
g_3 = \frac{y_3}{x - y_3 - 2y_4},
\]
\[
g_4 = \frac{y_4}{(1/2 - x - y_7 - 2y_4) (x - y_3 - 2y_4)},
\]
\[
g_7 = \frac{y_7}{1/2 - x - y_7 - 2y_4}.
\]  
\tag{17}

It should be mentioned that \(L^{-1} \ln R\) is rigorously a convex upwards function of \(y_3, y_4, y_7\) at any fixed \(x\). This means that, in effect, we search the maximum of a function of the only inexplicit variable.

To calculate the ground state energy of the Hamiltonian \(\[1\]\) we need to evaluate the density matrix of the first order using the trial function \(\[8\]\).

Here, there is a significant complication as compared to the Gutzwiller trial wave function. While a fermion hops from site \(i\) to site \(j\), the initial configurations of pair \(i - j\) and adjacent pairs \((i - k, j - l)\) change (see Fig.1a). Let us fix a configuration of pair \(i - j\) and adjacent pairs \(i - k, j - l\) and calculate function \(W\) of residual lattice by means of Eqs.\(\[1\]\), \(\[12\]\), and \(\[13\]\). The result is denoted by \(W'\). Then, a fraction of configurations containing the fixed fragment can be written as follows
\[
\frac{W'}{W} = y_{(ij)} \prod_k \left(\frac{y_{(ki)}}{x_{(i)}}\right) \prod_j \left(\frac{y_{(ij)}}{x_{(j)}}\right)
\]  
\tag{19}

where \(y_{(ij)}\) means some \(y_i\) corresponding to pair \((ij)\). The term of the density matrix which comes from the transition from configuration 1 to configuration 2 takes the form
\[
\frac{\prod_i g_i(2)}{\prod_i g_i(1)} \frac{W'(1)}{W}
\]  
\tag{20}

where the first factor is the ratio between amplitudes of configuration 1 and 2, i.e. \(g_i(1)\) and \(g_i(2)\) correspond to the configurations 1 and 2. In general, the procedure is similar to the Gutzwiller method \[8\] but the only parameter \(g_0\) enters into Eq.\(\[20\]\) in the latter case.

By means of Eqs. \(\[15\]\) and \(\[21\]\) one can sum up over all the configurations and calculate the density matrix
\[
\rho = 4 \left[2y_4 (a_1 a_2)^{z-1} + \frac{y_3 y_7 a_1^2 (z-1)}{g_0 g_3} + \frac{y_7 y_0 g_3}{g_7} a_2^{2(z-1)}\right],
\]  
\tag{21}

where
\[
a_1 = \frac{y_2 y_4 + y_3 y_4 g_3^{-1} + y_4 (g_7 + 1) g_4^{-1}}{x},
\]
and
\[
a_2 = \frac{y_6 y_4 + y_7 y_4 g_7^{-1} + y_4 (g_3 + 1) g_4^{-1}}{1/2 - x}.
\]

The first term of Eq.\(\[23\]\) describes transitions which do not change the total number of doubly occupied sites. The second and third terms are due to transitions corresponding to annihilation or creation of a doubly occupied site. Let us exclude parameters \(g_i\) by means of Eqs.\(\[17\]\). Then, after straightforward simplifications we obtain
\[
\rho = 8(y_4 + \sqrt{y_3 y_7}) \left[\frac{y_4}{x(1/2 - x)} \times (\sqrt{y_2 + \sqrt{y_3 + \sqrt{y_6 + \sqrt{y_7}}}})^{z-1}\right].
\]  
\tag{22}

Finally it is convenient to present the total energy of Fermi system in Gutzwiller’s form
\[ E = \frac{1}{L} \langle \psi | H | \psi \rangle = q\varepsilon_0 + xU \]  

(23)

where \( q = \rho / \rho^0 \), \( \rho^0 \) is the density matrix \( \rho \) at \( U = 0 \),

\[ \varepsilon_0 = 2V_F \int \varepsilon_k d\mathbf{k} \]

is the average energy of the non-interacting fermions. First we calculate \( \rho^0 \) by minimization of the ground state energy at \( U = 0 \), i.e. \( \rho^0 = \min_{\{x,y,z,y',z'y\}} \langle \rho \rangle \).

The ground state energy at nonzero \( U \) is determined by \( \min_{\{x,y,z,y',z'y\}} (E) \). The function \( E \) turns out to be smooth, without singular points within the domain of the function and its minimum is easily found numerically. I used a refined Nelder-Mead simplex algorithm for the minimum search.

The ground state energy of the PM phase calculated by this method is shown in Fig.2: (a) a one-dimensional chain \((z = 2)\) with the dispersion law \( \varepsilon_k = -2 \cos k_x \), (b) a square lattice \((z = 4)\), \( \varepsilon_k = -2(\cos k_x + \cos k_y) \), (c) a simple cubic lattice \((z = 6)\), \( \varepsilon_k = -2(\cos k_x + \cos k_y + \cos k_z) \). Symmetric and antisymmetric correlation functions of the nearest neighbors

\[ G_s = \langle n_1 n_2 \rangle + \langle n_1 n_2 \rangle = 2(y_2 + 2y_4 + y_6), \]

\[ G_a = \langle n_1 n_2 \rangle + \langle n_1 n_2 \rangle = 2(y_2 + 2y_4 + y_6) \]

(24)

are shown in Fig.3 for the same lattices as in Fig.2. The prime in Eqs.24 denotes the averaging over nearest-neighbor pairs only. Further details of the calculations can be found in Ref. [10]. This technique was also applied to the AFM phase of the Hubbard model [10].

C. Low-energy spectrum and effective mass

To investigate the energy spectrum of low-lying excitations in a model with the total energy of the form \( \langle \rho \rangle \), one can use the Fermi liquid approach of Ref. [26]. Let \( E_g \) be the ground state of the system \( \langle \rho \rangle \). Then, let us create a new initial state \( |\varphi_{k\sigma}\rangle = a_{p\sigma}^\dagger a_{p'\sigma}^\dagger |\varphi_0\rangle \) and a new trial wave function

\[ |\psi_{k\sigma}\rangle = \prod_{\lambda} g_{\lambda}^k |\varphi_{k\sigma}\rangle \]

(25)

where \( \mathbf{k} = \mathbf{p} - \mathbf{p}' \), \( \mathbf{p} \) and \( \mathbf{p}' \) are wave vectors lying above and below the Fermi surface, correspondingly. \( |\varphi_0\rangle \) is the ground state of non-interacting fermions. It should be noted that the new trial wave function has the same number of fermions of each spin as the initial wave function (the canonical ensemble). Since the operator on the right hand side of Eq.(16) is translationally invariant the new trial wave function has the well-defined wave vector \( \mathbf{k} \). Then, we perform the procedure developed above to determine the minimum energy \( E_g + \delta E_{k\sigma} \) corresponding to the excited state \( |\psi_{k\sigma}\rangle \), i.e. we find a new stationary solution of the Hamiltonian \( \langle \rho \rangle \). It is easy to see that \( \delta E_{k\sigma} \) is small, of the order of \( 1/N \). We express the energy variation as

\[ \delta E_{k\sigma} = q \delta E_0^{k\sigma} + \varepsilon_0 \left( \frac{\partial q}{\partial x} \right) + \sum_i \frac{\partial q}{\partial \lambda_i} \delta \lambda_i + U \delta x \]

(26)

where \( \lambda_i = y_3, y_4, y_7 \) and \( \delta E_0^{k\sigma} \) is the energy variation of non-interacting fermions corresponding to the excitation \( |\varphi_{k\sigma}\rangle \). Since the ground state is minimal the following conditions are valid

\[ \varepsilon_0 \frac{\partial q}{\partial x} + U = 0, \]

\[ \frac{\partial q}{\partial \lambda_i} = 0. \]

(27)

Combining Eqs.(26) and (27) we find that \( \delta E_{k\sigma} = q \delta E_0^{k\sigma} \) for any trial wave function generated by Eq.(25), i.e. the low-lying energy spectrum of our model is

\[ \varepsilon_{k\sigma} = q \varepsilon_0^{k\sigma} \]

where \( \varepsilon_0^{k\sigma} \) is the energy spectrum of non-interacting fermions. Retaining the terms of the second order infinitesimal in the expansion \( \langle \rho \rangle \) we obtain the effective Fermi liquid theory [26]. One can perform the similar calculation with the grand canonical ensemble \( \langle |\varphi_{k\sigma}\rangle = a_{p\sigma}^\dagger |\varphi_0\rangle \) but it would be more complicated because, in this case, a dependence of \( q \) on the number of fermions has to be taken into account. The effective mass at the Fermi surface is \( m = q^{-1} \) where the effective mass of non-interacting fermions is assumed to be \( m_0 = 1 \). This result is in an agreement with the phenomenological Brinkman-Rice approach [23] and slave-boson treatment [24]. The effective mass in the half-filled Hubbard model is shown in Fig.4 as a function of \( U \). A detailed discussion of the excitation spectrum will be presented elsewhere.

III. GROUND STATE OF THE KONDO-HUBBARD LATTICE

The Kondo-Hubbard lattice model can be expressed in the following form \( \langle \rho \rangle \)

\[ H_{KH} = H_H + J \sum_i \mathbf{S}_i^c \mathbf{S}_i^c = H_H + J \sum_i \left[ S_{i+}^d S_{i-}^c + \frac{1}{2} \left( S_{i+}^d S_{i-}^c + S_{i-}^d S_{i+}^c \right) \right], \]

(28)

where \( H_H \) is the Hubbard Hamiltonian, \( \mathbf{S}_i^c \) is the spin operator of an itinerant fermion at site \( i \), \( \mathbf{S}_i^d \) denotes the spin of the total angular moment operator (f-spin) depending on the nature of the localized state. We consider the PM phase at half band-filling. It is convenient to represent the Kondo-Hubbard lattice as an equivalent lattice
in Fig.1b. Here, we obtain a new sort of nearest-neighbor pairs, namely, itinerant fermion - localized fermion on the same site (open circle - black circle in Fig.1b). It should be noted that there are no additional closed paths in the lattice as compared to Fig.1a. That is why, we don’t bring about additional simplifications as compared to the Hubbard model. The general form of the trial wave function of the Kondo-Hubbard lattice can be presented as

\[ |\psi^{KH}\rangle = \tilde{g}_r^{\uparrow} |\psi^H\rangle |\varphi_{\uparrow}\rangle = g_r^{\uparrow} \prod_{\lambda} \tilde{g}_{\lambda}^{\uparrow} |\varphi_{\uparrow}\rangle |\varphi_{\uparrow}\rangle \] (29)

where |\varphi_{\uparrow}\rangle\rangle is the initial wave function of itinerant (c) and localized fermions (l), \( \tilde{g}_r \) are the projection operators for the Hubbard model \( \langle \tilde{H} \rangle \), |\psi^H\rangle is the trial wave function of the Hubbard model and \( \tilde{g} = -4 \sum_{\nu} S_{\nu}^L S_{\nu}^C \) is the new projection operators for itinerant fermion - localized fermion pairs. Index z denotes the projection on z-axis. |\varphi\rangle is the PM phase without correlations (all spin configurations are equiprobable). In the next two subsections, we shall define concretely the trial wave function \( \langle 29 \rangle \) for two cases.

### A. S = 1/2 Kondo-Hubbard lattice

There are three eigenstates of operator \( S^{L}_{r} S^{C}_{r} \) in case of the spin 1/2 localized state (singlet, triplet and \( S^{C}_{r} = 0 \), see Table 1). Let us introduce the eigenvalues of the operator \( r_0, r_1 \) and \( r_2 \). The self-consistency and normalization conditions \( \langle \tilde{H}\rangle \), \( \langle \rangle \) remain valid and new ones appear

\[ r_0 = x, \quad r_1 + r_2 = 1/2 - x. \] (30)

From this it follows that a new independent parameter \( r = r_1 \) appears in addition to the set describing the Hubbard subsystem \( (x, y_3, y_4, y_7) \). Then, the trial wave function takes the form

\[ |\psi^{KH}\rangle = \tilde{g}_r^{\uparrow} |\psi^H\rangle |\varphi_{\uparrow}\rangle = g_r^{\uparrow} \tilde{g}_r \tilde{g}_r^{\uparrow} \tilde{g}_3 \tilde{g}_3^{\uparrow} \tilde{g}_4 \tilde{g}_4^{\uparrow} \tilde{g}_7 \tilde{g}_7^{\uparrow} |\varphi_{\uparrow}\rangle |\varphi_{\uparrow}\rangle . \] (31)

and its norm is

\[ \langle \psi | \psi \rangle = \sum_{\{r, x, y_3, y_4, y_7\}} W^K_{\{r, x\}} W^H_{\{x, y_3, y_4, y_7\}} \times g_r^{\uparrow} \tilde{g}_r \tilde{g}_r^{\uparrow} \tilde{g}_3 \tilde{g}_3^{\uparrow} \tilde{g}_4 \tilde{g}_4^{\uparrow} \tilde{g}_7 \tilde{g}_7^{\uparrow} = \sum_{\{r, x, y_3, y_4, y_7\}} R_{\{r, x, y_3, y_4, y_7\}} \] (32)

where \( W^K(H) \) is the Kondo (Hubbard) weight of the set. \( W^H \) is from Eqs. (23) and (24). The Kondo weight can be easily calculated

\[ W^K = \frac{(2rL)!}{(xL)!} \left( \frac{[L(1/2 - x)!]}{[rL]!(L(1/2 - x - r)!)} \right)^2 . \] (33)

Using Eqs. (32) and (33) we search the global maximum of the norm following the procedure described in the previous section. We obtain the system of equations \( \{16\} \) where \( y_3 = r, y_4, y_5, y_7 \). The equations for parameters \( g_1, g_4 \) and \( g_7 \) remain the same as in system \( \{17\} \). For the other parameters we obtain

\[ g_r \frac{1}{2} \left( \frac{1/2 - x}{x} \right) \left( \frac{x - y_3 - 2y_4}{1/2 - x - y_7 - 2y_4} \right)^{1/2} , \] (34)

The total energy of the Kondo-Hubbard lattice includes Hubbard and exchange parts

\[ E = \frac{1}{L} \langle \psi | H | \psi \rangle = q \varepsilon_0 + xU + J(\rho_{zz} + \rho_{\pm}) \] (35)

where \( q = \rho_H / \rho_H^0, \rho_H^0 \) is the Hubbard density matrix at \( U = 0, \rho_{zz}, \rho_{\pm} \) are the density matrices corresponding to \( zz \) and spin-flip interactions. Since there are new bonds in the lattice in Fig.1b, the Hubbard density matrix is different from that of the Hubbard model. Thus, instead of Eq. (21) we get

\[ \rho_H = \left[ \begin{array}{ccc} 2y_4 a_1 a_2 & 1/2 & b_2 \\ 0 & 1/2 & b_2 \\ 0 & 1/2 & b_2 \end{array} \right] \] (36)

where

\[ b_1 = r g_r^{-1} + g_r (1/2 - x - r) , \]
\[ b_2 = \frac{1}{2} \left( g_r + g_r^{-1} \right) . \]

Straightforward calculations of exchange terms give

\[ \rho_{zz} = -\frac{1}{2} (2r + x - 1/2) , \] (37)
\[ \rho_{\pm} = -2y_4 + y_6 y_7 + y_7 g_r^{-1} . \]

Expressions (35), (36) and (37) present the total energy of the Kondo-Hubbard lattice in an analytic form as a function of independent variational parameters \( r, x, y_3, y_4, y_7 \). The ground state energy is the global minimum of Eq. (35) with respect to these parameters. The spin nearest-neighbor correlation function of the itinerant subsystem

\[ G_c = \langle S_{zz}^{(1)} S_{zz}^{(2)} \rangle = (G_x - G_a) / 4 = \frac{1}{2} (y_6 - y_7) \] (38)

and the spin correlation function of localized nearest neighbors are shown in Fig.5. The last is calculated by means of the superposition hypothesis \( \{22\} \).
\[
G_t = \langle S^c_{z_1} S^c_{z_2} \rangle \left[ \langle S^c_{z_1} S^t_{z_1} \rangle \right]^2
= \frac{1}{2} (1 - 2x - 4r^2) (y_b - y_r). \tag{39}
\]

Following the expansion [29], we determine the effective mass of the itinerant fermions as \( m = q^{-1} \). It is plotted against \( J \) in Fig.6. We have also plotted the fraction of lattice sites occurred to be in the Kondo singlet state (2r) in Fig.7.

B. \( S = 5/2 \) Kondo-Hubbard lattice

Bearing in mind cerium Kondo-Hubbard lattices (Ce\(^{3+}\)) we generalize the technique developed above to spin 5/2 (the total angular moment or \( f \)-spin). The crystal field is neglected in the Hamiltonian [29]. Crystal field effects will be discussed briefly in the next section. Let us compile a table of all intrasite configurations (see Table [11]). Since the Hamiltonian [29] is rotation invariant, possibilities of configurations with \( S_{iz}^c = 0 \) are equal each other, \( r_0 = x/3 \). There are 6 configurations with \( S_{iz}^c \neq 0 \). They are bound by the normalization condition

\[
\sum_{i=1}^{6} r_i = 1/2 - x. \tag{40}
\]

It follows that one of \( r_i \) is dependent (we take \( r_6 \) as the dependent parameter). The general trial wave function [31] remain valid for the spin 5/2. Then, its norm is

\[
\langle \psi | \psi \rangle = \sum_{\{r_i, x, y_3, y_4, y_7\}} W^K_{\{r_i, x\}} W^H_{\{x, y_3, y_4, y_7\}}
\times g_r^4 L \sum_{i=1}^{6} r_i (7 - 2i) g_0^2 L x_3 y_3 2 z L y_5 8 z L y_4 y_4 2 z L y_7. \tag{41}
\]

In case of \( S = 5/2 \), the Kondo part of the configuration weight is reduced to

\[
W^K = \frac{(2xL)!}{[(xL)!]^5} \left( \prod_i (r_i L)! \right)^2. \tag{42}
\]

The necessary condition of the global maximum of \( R [40] \), where \( \eta_\lambda = r_i, x, y_3, y_4, y_7 \), leads to a system of nine equations. In particular, there are five equations for independent \( r_i \)

\[
g_r^{2(12-2i)} = \frac{r_i}{r_6}. \tag{43}
\]

where \( r_6 = 1/2 - x - \sum r_i \). From here one can see that, in effect, there is the only independent parameter \( r \). Let it be \( r = r_1 \). This is no wonder because the only variational parameter \( r \) enters into the trial wave function. The five equations for \( r_i \) gives the nonlinear equation relating \( r \) and \( g_r \)

\[
r \left( 1 + g_r^{-4} + g_r^{-8} + g_r^{-12} + g_r^{-16} + g_r^{-20} \right) = 1/2 - x, \tag{44}
\]

The equation for \( g_0 \) transforms to

\[
g_0 = \frac{1/2 - x}{6 \sqrt{1 + r}} \left( \frac{1/2 - x}{x} \right)^{z^{-1}} \times \left( \frac{x - y_3 - 2y_4}{1/2 - x - y_r - 2y_4} \right)^{z/2}. \tag{45}
\]

The equations for \( y_3, y_4, y_7 \) are the same as for the Hubbard model [17].

The density matrix falls into the Hubbard, \( zz \) and spin-flip terms in the same manner as for the localized spin 1/2. The general form of the Hubbard term is Eq.(39) where

\[
b_1 = \frac{1}{6} \sum_{i=1}^{3} (g_r^{2i-1} + g_r^{1-2i}) ,
\]

\[
b_2 = \frac{r}{1/2 - x} \sum_{i=1}^{6} g_r^{-3-2i}.
\]

Straightforward calculations give the \( zz \) and spin-flip terms

\[
\rho_{zz} = -\frac{1}{2} \sum_{i=1}^{6} r g_r^{4(1-i)} (7 - 2i), \tag{46}
\]

\[
\rho_{\pm} = -(1 - 2x - r g_r^{-20}) g_r^{-2}. \tag{47}
\]

The total energy is written in the form of Eq.(33). The ground state energy is determined by the minimization over the independent variational parameters. There is a complication of the numerical procedure because in the present case the variational parameter \( g_r \) can’t be expressed analytically in terms of \( r \). In other respects the calculations are similar to that discussed in previous sections. The spin correlation function of itinerant fermions [33] and that of localized states

\[
G_t = \langle S^c_{z_1} S^c_{z_2} \rangle \left[ \langle S^c_{z_1} S^t_{z_1} \rangle \right]^2
= \frac{1}{4} (y_b - y_r) r^2
\times (5 [1 - g_r^{-20}] + 3 [g_r^{-4} - g_r^{-16}] + g_r^{-8} - g_r^{-12}) \tag{47}
\]

are shown in the insert in Fig.5. The effective mass and the function 2r are plotted in the inserts in Fig.6 and Fig.7.

IV. DISCUSSION AND CONCLUSIONS

The trial wave functions used in the present approach [3], [29] have a remarkable property. The operator on the right side of Eq.(3) commutes with the operators of the crystal point group (rotations, reflections, inversion) and the translation group. That is why the trial wave function retains all the symmetries of the initial wave function. In contrast to the Gutzwiller wave function, we
have incorporated the nearest-neighbor correlations into the trial wave function. That is why, a local structure surrounding an atom appears. A similar trial wave function was used in Ref. [13]. The ground state energy was evaluated there by means of an expansion of exponent \( \exp(-\gamma \tilde{Y}_\lambda) \). To perform this a systematic diagram representation was introduced [13]. This approach turned out to be very successful in quantum chemistry for small molecules because one obtains an excellent results taking into account the first terms of the series. At the same time, the eigenvalues of \( \tilde{Y}_\lambda \) are approximately proportional to the number of lattice sites. That is why, it is hardly possible to use this approach in the thermodynamic limit \( (L \to \infty) \) for the strong short-range order. Let us consider a set of approximations in the framework of Kikuchi’s method, namely the Gutzwiller approximation (a cluster consists of the only site) as the first one, a pair Kikuchi’s approximation (a cluster consists of two sites) as the second one, and etc. On each step, a cluster becomes larger. It was rigorously proved for 2D square lattice and 3D cubic lattice that in the thermodynamic limit we approach the rigorous solution while a cluster size increases [27]. This allows us to go beyond the infinite dimension limit.

We calculated the ground state energy of the Hubbard model in the PM phase for a one-dimensional chain, square and simple cubic lattices (see Fig.2). The result for a one-dimensional chain is very close to that obtained by an analytic investigation of Gutzwiller wave function [24]. Let us mention that the method presented above gives much lower the ground state energy in the AFM phase [16]. The results for the square and simple cubic lattices are compared with that of the VMC method [17] in Fig.2b,c. Since the VMC method is based on the Gutzwiller trial wave function the difference between this approach and our method is due to effects of the short-range correlations. It can be seen that near \( Uc = 8 |z_0| \) (i.e. the critical value of \( U \) in the Gutzwiller approximation) the ground state energy of the trial wave function Eq.(8) is substantially lower (two or three times) than that obtained by the VMC method, i.e. the short-range order considerably reduces the ground state energy. This result is in contrast to the 1/D-expansion in the dynamical mean field theory [13] and shows that the perturbation theory methods are hardly suitable here.

The narrow quasi-particle band (see Fig.4) is appeared at the Fermi level similarly to the results of Gutzwiller’s approach [12]. At large \( U \), the effective mass become linear on \( U \). The slope of the function \( m(U) \) increases while the lattice dimension becomes larger. The limit of infinite dimensions of the ground state [8] was investigated in Ref. [19]. While the lattice dimension increases, the ground state energy approaches to Gutzwiller’s solution. We also note that an exchange hole exists in the variational solution even at \( U = 0 \) \( (G_s < 0.5) \). It increases monotonically while \( U \) grows (exchange-correlation hole). Unlike the well-known Hubbard III solution the short-range AFM correlations do not disappear in the limit \(|t|/U \ll 1\) but tend to a certain constant value (see Fig.3). In this limit, the Hubbard model at half band-filling reduces to the spin-1/2 Hiesenberg model. The residual AFM correlations in the PM phase are consistent with the results of the ground state studying of the Hiesenberg model [23]. It was also shown in Ref. [16] that in the AFM phase, the both methods (the VMC method and the present one) give almost the same ground state energy, i.e. in the presence of the long-range order, the short-range correlations are inessential.

In the Kondo-Hubbard model we observe two different types of behavior depending on value of \( J \). At small \( J \), the exchange term weakly affects the ground state energy and effective mass. It should be noted that the AFM correlations between localized states at a pair of nearest-neighbors sites \( (G_l) \) increase with increasing of \( J \). This effect appears because the short-range AFM correlations between band fermions exist at \( J = 0 \) and at small \( J \) the correlations between localized states follow the correlations of band fermions. The growth of the exchange leads to suppression of the band correlations. In Fig.5, it is seen a transition to another regime (large \( J \)). For simple cubic lattice we have obtained a discontinuity of \( G_c \) and a sharp turn of \( G_l \) for both \( S^l = 1/2 \) and \( S^l = 5/2 \) cases, i.e. a phase transition. A smooth crossover is observed in 1D chain and square lattice at this point (see Fig.5). At present, it is hardly possible to establish a kind of the phase transition. We can rule out the first order transition only because the ground state energy is smooth (the derivative of the ground state energy is continuous). At higher \( J \), the correlations between localized states start to decrease with increasing \( J \). It should be mentioned that the behavior of the spin correlation function \( G_l \) is similar to that ensued from Doniach’s phase diagram despite the fact that the RKKY interaction is not included into the variational theory.

The Coulomb interaction between itinerant fermions \( U \) influences the ground state in two ways. On the first hand, it reinforces the short-range order and increases the AFM correlations between nearest-neighbor localized states. On the other hand, at large \( U \) the effective quasi-particle band gets smaller that favors the Kondo regime. At large \( J \), the ground state energy approaches asymptotically the energy of the pair singlet state \((\frac{J}{2} J)\) for \( S^l = 1/2 \). The probability of the Kondo singlet \((2r)\) at a site goes to 1 (see Fig.7) for \( S^l = 1/2 \) and to some fixed value (independent on the lattice dimension) for \( S^l = 5/2 \). The difference is due to the fact that, in the first case, the ground state is a superposition of two antiparallel states \((\frac{1}{\sqrt{2}} (|↑↓⟩ − |↓↑⟩))\) and, in the case of a pair \( S^l = 5/2, S^c = 1/2 \), it involves all the possible states \((|S^l_{zi} = \frac{5}{2}⟩ |S^c_{zi} = -\frac{1}{2}⟩, |S^l_{zi} = \frac{3}{2}⟩ |S^c_{zi} = -\frac{3}{2}⟩ \) and etc.) for the total energy to be minimal. At large \( J \) the effective mass of itinerant fermions increases drastically and tends to almost linear behavior with variation \( J \) \((m \propto \alpha J)\) where \( \alpha \) is the constant depending on the type
of lattice) as can be seen in Fig.6. This is the Kondo lattice regime. In the case of $S^I = 5/2$, the effective mass is significantly larger than for $S^I = 1/2$. In a real system, $n$ can’t increase infinitely and a localization of fermions should occur due to disorder or temperature effects but this is beyond the scope of the present paper.

The crystal field can be taken into account in the variational scheme. It can be easily done in the limit of the strong crystal field when we consider the lowest level of the multiplet only. In the general case, we have to use additional variational parameters to control different populations at multiplet levels. For instance, if the ground state of Ce$^{3+}$ ion is splitted by the crystal field into a doublet and a quadruplet (e.g. $\Gamma_7$ and $\Gamma_8$ states), we should apply the only additional variational parameter to the trial wave function. If it is splitted into three doublets, we have to use two additional parameters and etc.

In the framework of the variational theory presented above the strongly correlated coherent metal state appears in a natural way similarly to the Gutzwiller theory. This provides a good basis for investigations of strongly correlated systems and dense Kondo systems by means of this theory. The main shortcoming of our approach is neglect of closed loops while we treat the correlations on a lattice. Nevertheless, it is considered that Kikuchi’s method yields a good approximation if the correlation length is not greater than a cluster size [29]. The well-developed cluster variation method allows to include short closed loops, which are most important, into considerations [30]. The short-range correlations are observed directly by the neutron scattering. The AFM correlations in the strongly correlated metals like V$_2$O$_3$ and Kondo lattices turn out to be strong but very short [25]. That is why the closed loops are inessential in this substances. Let us mention that one can calculated the neutron cross-section and dynamical susceptibility of these results obtained above. At the same time, it is hardly possible to apply the present theory to systems with lengthy AFM correlations (e.g. strongly underdoped high temperature superconductors [3]).

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VI. FIGURE CAPTIONS

Fig.1. (a) A fragment of $z = 4$ lattice, (b) representation of $z = 4$ Kondo-lattice. Itinerant and localized states are shown as light and black circles, correspondingly; double lines denote the exchange interaction.

Fig.2. The ground state energy of the Hubbard model at half-band filling. (a) A one-dimensional chain: the...
Gutzwiller solution (1), present study (2), the exact solution; (b) square and (c) simple cubic lattices: the Gutzwiller solution (1), the VMC method (2), the present study (3).

Fig. 3. The symmetric $G_s$ (dashed lines) and antisymmetric $G_a$ (solid lines) correlation functions of the Hubbard model for a one-dimensional chain (1), square (2) and simple cubic lattices (3).

Fig. 4. The effective mass in the half-filled Hubbard model: a one-dimensional chain (1), square (2) and simple cubic lattices (3). The dashed lines are guides to eye.

Fig. 5. The spin correlation functions $G_c$ (dashed lines) and $G_l$ (solid lines) for the half-filled $S = 1/2$ Kondo-Hubbard model: (a) a one-dimensional chain, (b) square and (c) simple cubic lattices; $U = 0.5 U_c$. The correlation functions for the half-filled $S = 5/2$ Kondo-Hubbard model are shown in the insert.

Fig. 6. The effective mass in the $S = 1/2$ Kondo-Hubbard model: a one-dimensional chain (1), square (2) and simple cubic lattices (3); $U = 0.5 U_c$. The dashed lines are guides to eye. The effective mass for the half-filled $S = 5/2$ Kondo-Hubbard model is shown in the insert.

Fig. 7. The probability of the Kondo singlet state in the $S = 1/2$ Kondo-Hubbard model (2r). The probability of $|S_{zi}^c = \pm 5/2 \rangle |S_{zi}^c = \mp 1/2 \rangle$ states in the $S = 5/2$ Kondo-Hubbard model is shown in the insert.

TABLE I. Pair projection operators, corresponding configurations and the degeneracy factor

| Operator | Configuration | Degeneracy |
|----------|---------------|------------|
| $\tilde{Y}_1$ | ↑ ↓ | 1 |
| $\tilde{Y}_2$ | ↑ ↓ | 1 |
| $\tilde{Y}_3$ | ↑ ↓ | 2 |
| $\tilde{Y}_4$ | ↑ | 2 |
| $\tilde{Y}_5$ | ↓ | 2 |
| $\tilde{Y}_6$ | ↑ ↑ | 1 |
| $\tilde{Y}_7$ | ↑ | 2 |
| $\tilde{Y}_8$ | ↑ ↓ | 2 |
| $\tilde{Y}_9$ | ↑ ↓ | 2 |
| $\tilde{Y}_{10}$ | ↓ ↓ | 1 |

TABLE II. Intrasite configurations of the spin 1/2 Kondo-Hubbard lattice

| Configuration | Eigenvalue | Degeneracy |
|---------------|------------|------------|
| Itinerant state $S_z^{it}$ | Localized state $J_z^{it}$ | $\beta_i$ |
| $S = 0$ | ↑ | $x$ | 2 |
| ↑ | ↑ | $1/2 - r - x$ | 2 |
| ↑ | ↓ | $r$ | 2 |

TABLE III. Intrasite configurations of the spin 5/2 Kondo-Hubbard lattice

| Configuration | Eigenvalue | Degeneracy |
|---------------|------------|------------|
| Itinerant state $S_z^{it}$ | Localized state $J_z^{it}$ | $\beta_i$ |
| 0 | any state | $x$ | 2 |
| 1/2 | −5/2 | $r_1$ | 2 |
| 1/2 | −3/2 | $r_2$ | 2 |
| 1/2 | −1/2 | $r_3$ | 2 |
| 1/2 | 1/2 | $r_4$ | 2 |
| 1/2 | 3/2 | $r_5$ | 2 |
| 1/2 | 5/2 | $r_6 = 1/2 - x$ | 2 |
| $\sum_{i=1}^5 r_i$ | | | |
