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EXACT SINGLET BOND GROUND STATES FOR ELECTRONIC MODELS

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We proposed several 1D and 2D electronic models with the exact ground state. The ground state wave function of these models is represented in terms of 'singlet bond' functions consisting of homopolar and ionic configurations. The Hamiltonians of these models include correlated hopping of electrons, pair hopping terms and spin interactions.

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The study of strongly correlated electron systems has been an important subject in theoretical condensed matter physics. In general, the Hamiltonians of these systems include many types of interactions, and they are difficult to solve. The integrable models provided us a very good understanding of correlation effects in many-body systems. Unfortunately, the construction of such models is difficult due to the strict conditions for the integrability. In recent years there has been increasing interest in studying models where at least the ground state can be found exactly [1 – 4]. The most popular methods for the construction of an exact ground state are the so-called optimal ground state (OGS) approach [2] and the matrix-product (MP) method [3, 4]. The ground state wave function in the MP method is represented by *Trace* of a product of matrices describing single-site states. This ground state is 'optimal' in the sense that it is the ground state of each local interaction. This method allows to construct a large class of spin models. The similar approach has been used in the OGS method for the construction of the electronic models with the special ground states.

In this paper we propose new 1D and 2D models of interacting electrons with an exact ground state. We note that our models have ground states which are very different from those constructed in the OGS approach. The ground state wave function of our models is expressed in terms of the two-particle *'singlet bond'* (SB) function located on sites i and j of the lattice:

$$[i,j] = c^+_{i,\uparrow}c^+_{j,\downarrow} - c^+_{i,\downarrow}c^+_{j,\uparrow} + x\,(c^+_{i,\uparrow}c^+_{i,\downarrow} + c^+_{j,\uparrow}c^+_{j,\downarrow})\,|0\rangle\,, \qquad (1)$$

where $c^+_{i,\sigma}$, $c_{i,\sigma}$ are the Fermi operators and x is an arbitrary coefficient. The SB function is the generalization of the Resonating Valence Bond (RVB) function [5] including ionic states. The presence of the ionic states is very important from the physical point of view because, as a rule, the bond functions contain definite amount of the ionic states as well.

It is known a set of 1D and 2D quantum spin models the exact ground state of which can be represented in the RVB form [6 – 10]. It is natural to try to find electronic models with exact ground state at half-filling formed by SB functions in the same manner as for

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above mentioned spin models. The electronic models of these types include the correlated hopping of electrons as well as the spin interactions and pair hopping terms.

The model with dimerization. As the first example we consider the 1D electronic model with the two-fold degenerate ground state in the form of the simple product of SB dimers, similarly to the ground state of the well-known spin-1/2 Majumdar-Ghosh model [6]. For the half-filling case the proposed ground state wave functions are:

$$\Psi_1 = [1,2][3,4]...[N-1,N] \tag{2}$$

and

$$\Psi_2 = [2,3][4,5]...[N,1]. \tag{3}$$

In order to find the Hamiltonian for which the wave functions (2) and (3) are the exact ground state wave functions, we represent the Hamiltonian as a sum of local Hamiltonians h_i defined on three neighboring sites (periodic boundary conditions are supposed):

$$H = \sum_{i=1}^{N} h_i. \tag{4}$$

The basis of three-site local Hamiltonians h_i consists of 64 states, while only eight of them are present in Ψ_1 and Ψ_2. These 8 states are

$$[i,i+1]\,\varphi_{i+2}, \qquad \varphi_i\,[i+1,i+2], \tag{5}$$

where φ_i is one of four possible electronic states of i-th site: $|0\rangle_i$, $|\uparrow\rangle_i$, $|\downarrow\rangle_i$, $|2\rangle_i$.

The local Hamiltonian h_i for which all the functions (5) are the exact ground state wave functions can be written as the sum of the projectors onto other 56 states $|\chi_k\rangle$:

$$h_i = \sum_k \lambda_k \,|\chi_k\rangle\,\langle\chi_k|\,, \tag{6}$$

where λ_k are arbitrary positive coefficients. This means that the wave functions Ψ_1 and Ψ_2 are the ground states of each local Hamiltonian with zero energy. Hence, Ψ_1 and Ψ_2 are the 'optimal' ground state wave functions of the total Hamiltonian H with zero energy, similarly to the models in [2–4]. In general case, the local Hamiltonian h_i is many-parametrical and depends on parameters λ_k and x. We consider one of the simplest forms of h_i including the correlated hopping of electrons of different types and spin interactions between nearest- and next-nearest neighbor sites:

$$\begin{aligned} h_i &= 2 - x\,(t_{i,i+1} + t_{i+1,i+2}) + \\ &+ (x^2 - (1+x^2)(1-n_{i+1})^2)\,T_{i,i+2} + \\ &+ 8\frac{1-x^2}{3}(\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \mathbf{S}_{i+1} \cdot \mathbf{S}_{i+2} + \mathbf{S}_i \cdot \mathbf{S}_{i+2}), \end{aligned} \tag{7}$$

where

$$\begin{aligned} T_{i,j} &= \sum_\sigma (c^+_{i,\sigma} c_{j,\sigma} + c^+_{j,\sigma} c_{i,\sigma})(1 - n_{i,-\sigma} - n_{j,-\sigma}), \\ t_{i,j} &= \sum_\sigma (c^+_{i,\sigma} c_{j,\sigma} + c^+_{j,\sigma} c_{i,\sigma})(n_{i,-\sigma} - n_{j,-\sigma})^2 \end{aligned}$$

and $-_i$ is the $SU(2)$ spin operator.

Each local Hamiltonian h_i is a non-negatively defined operator at $|x| \leq 1$. The following statements related to the Hamiltonian (7) are valid.

1. The functions (2) and (3) are the only two ground state wave functions of the Hamiltonian (7) at $N_e = N$ (N_e is the total number of electrons). They are not orthogonal, but their overlap is $\sim e^{-N}$ at $N \gg 1$.

2. The ground state energy $E_0(N_e/N)$ is a symmetrical function with respect to the point $N_e/N = 1$ and has a global minimum $E_0 = 0$ at $N_e/N = 1$.

3. The translational symmetry of (7) is spontaneously broken in the ground state leading to the dimerization:

$$\langle |t_{i,i+1} - t_{i+1,i+2}| \rangle = 2.$$

The excited states of the model can not be calculated exactly but we expect that there has to be a gap, because the ground state is formed by the ultrashort-range SB functions. If it is the case, the function $E_0(N_e/N)$ has a cusp at $N_e/N = 1$.

Actually, this model is the fermion version of the Majumdar – Ghosh spin model. Moreover, it reduces to the Majumdar – Ghosh model at $x = 0$ and in the subspace with $n_i = 1$.

For $x = 1$ the Hamiltonian (7) simplifies and takes the form:

$$H = -2\sum_j (t_{j,j+1} - 1) - \sum_j e^{i\pi n_{j+1}} T_{j,j+2}. \tag{8}$$

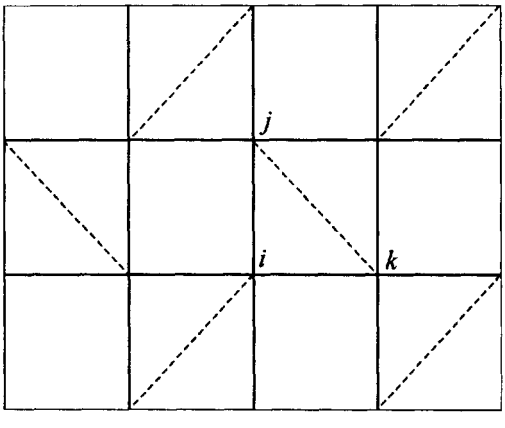

Fig.1. The lattice of the Shastry – Sutherland model

The 2D model. We can easily construct the 2D electronic model with the exact ground state which is analogous to the Shastry – Sutherland model [7] (Fig.1). The Hamiltonian of this model is:

$$H = \sum_{\{i,j,k\}} h_{i,j} + h_{i,k} + h^d_{j,k}, \tag{9}$$

where the sum is over all triangles $\{i, j, k\}$, one of which is shown on Fig.1. So, each diagonal line belongs to the two different triangles. The local Hamiltonians $h^d_{j,k}$ acting on the diagonal of the triangle $\{i, j, k\}$, and $h_{i,j}$, $h_{i,k}$ have the form (for the sake of simplicity we put $x = 1$)

$$h^d_{j,k} = -2\, t_{j,k} + 4,$$

$$h_{i,j} = -t_{i,j} - e^{i\pi n_k}\, T_{i,j},$$
$$h_{i,k} = -t_{i,k} - e^{i\pi n_j}\, T_{i,k}.$$

It is easy to check that

$$h^d_{j,k}\ |\varphi_i\,[j,k]\rangle = (h_{i,j} + h_{i,k})\ |\varphi_i\,[j,k]\rangle = 0.$$

All other states of the local Hamiltonian $h_{i,j} + h_{i,k} + h^d_{j,k}$ have higher energies. Therefore, the ground state wave function in the half-filling case is the product of the SB functions located on the diagonals shown by dashed lines on Fig.1. This model has non-degenerate singlet ground state with ultrashort-range correlations.

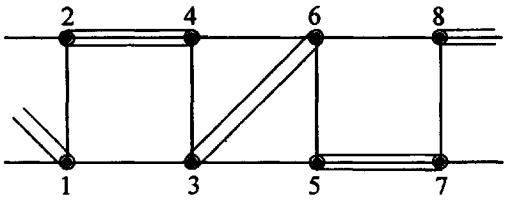

Fig.2. The two-leg ladder model

The ladder model. Let us now consider electronic models with a more complicated ground state including different configurations of short-range SB functions. The form of these ground states is similar to that for spin models proposed in [8] and generalized in [9]. In the 1D case our model describes two-leg ladder model (Fig.2). Its ground state is a superposition of the SB functions where each pair of nearest neighbor rungs of the ladder is connected by one SB. One of possible configurations of singlet bonds is shown on Fig.2.

The wave function of this ground state can be written as:

$$\Psi_s = \psi^{\lambda\mu}(1) g_{\mu\nu} \psi^{\nu\rho}(2) g_{\rho\kappa} \ldots \psi^{\sigma\tau}(N) g_{\tau\lambda}. \tag{10}$$

The wave function of this type for spin models has been proposed in [8]. The functions $\psi^{\lambda\mu}(i)$ describes i-th rung of the ladder

$$\psi^{\lambda\mu}(i) = c_1 \varphi^{\lambda}_{2i-1} \varphi^{\mu}_{2i} + c_2 \varphi^{\lambda}_{2i} \varphi^{\mu}_{2i-1} \tag{11}$$

with

$$\varphi^{\lambda}_k = \begin{pmatrix} |\uparrow\rangle_k \\ |\downarrow\rangle_k \\ |2\rangle_k \\ |0\rangle_k \end{pmatrix}, \qquad g_{\lambda\mu} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & x \\ 0 & 0 & x & 0 \end{pmatrix}$$

It is easy to see that

$$g_{\lambda\mu} \varphi^{\lambda}_i \varphi^{\mu}_j = [i,j].$$

Therefore, the function Ψ_s is a singlet wave function depending on two parameters x and c_1/c_2. Actually, this form of Ψ_s is equivalent to the MP form with 4×4 matrices $A_{\lambda\nu}(i) = g_{\lambda\mu}\psi^{\mu\nu}(i)$. Moreover, at $x = 0$ and $c_1/c_2 = -1$ the function Ψ_s reduces to the wave function of the well-known AKLT (Affleck, Kennedy, Lieb and Tasaki) spin-1 model [8].

In order to find the Hamiltonian for which the wave function (10) is the exact ground state wave function, it is necessary to consider what states are present on the two nearest

rungs in the Ψ_s. It turns out that there are only 16 states from the total 256 ones in the product $\psi^{\lambda\mu}(i)g_{\mu\nu}\psi^{\nu\rho}(i+1)$. The local Hamiltonian h_i acting on two nearest rungs i and $i+1$ can be written in the form of (6) with the projectors onto the 240 missing states. The total Hamiltonian is the sum of local ones (4). The explicit form of this Hamiltonian is very cumbersome and, therefore, it is not given here.

The correlation functions in the ground state (10) can be calculated exactly in the same manner as it was done for spin models [8]. It can be shown that all of correlations exponentially decay in the ground state. We expect also that this model has a gap.

This method of construction of the exact ground state can be generalized also to 2D and 3D lattices [9]. Following [9], one can rigorously prove that the ground state of these models is always a non-degenerate singlet.

1D models with the giant spiral order. There is one more spin-1/2 model with an exact ground state of the RVB type [10]. Its Hamiltonian has the form

$$H = -\sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{4}\sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+2} \tag{12}$$

This model describes the ferromagnet–antiferromagnet transition point. The exact singlet ground state can be expressed by the combinations of the RVB functions (i,j) distributed uniformly over the lattice points:

$$\Phi_0 = \sum (i,j)(k,l)(m,n)\dots \ , \tag{13}$$

where the summation is done over all combinations of sites under the condition that $i<j,\ k<l,\ m<n\dots$. The spin correlations in the singlet ground state show giant spiral structure [10].

The analog of the wave function (13) in the SB terms is:

$$\Psi_0 = \sum_{i<j\dots} (-1)^P\ [i,j][k,l][m,n]\dots, \tag{14}$$

where $P=(i,j,k,l,\dots)$ is the permutation of numbers $(1,2,\dots N)$. It is interesting to note that the singlet wave function (14) can be also written in the MP form but with an infinite size matrices [11]. The Hamiltonian for which the wave function (14) is the exact ground state wave function has a form:

$$H = \sum_{i=1}^{N} \left(T_{i,i+1} - \frac{2}{x} t_{i,i+1} - 4\,\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{4}{x^2}\eta_i \cdot \eta_{i+1} + 4\,\frac{x^2-3}{x^2}\eta_i^z \eta_{i+1}^z \right), \tag{15}$$

where

$$\eta_i^+ = c_{i,\downarrow}^+ c_{i,\uparrow}^+, \qquad \eta_i^- = c_{i,\uparrow}\, c_{i,\downarrow}, \qquad \eta_i^z = (1-n_i)/2.$$

This model describes the transition point where the singlet ground state (14) is degenerate with ferromagnetic state. The spin-spin correlations in the singlet ground state (14) have a giant spiral form, as in the spin model (12), while other correlations vanish in the thermodynamic limit [11].

In summary, we have constructed electronic models with an exact ground state. The ground state wave function of these models is built from SB functions in the same manner as the well-known RVB ground states of spin models. We have considered three types of

SB ground states. All of considered electronic models have similar physical properties as the original spin models. We note that the proposed approach can be generalized for the construction of other models with the ground states of more complicated SB forms.

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