Exact Resonating-Valence-Bond Ground State and Possibility of Superconductivity in Repulsive Hubbard Models

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We generalize the exactly solvable Hubbard model with infinitely large on-site Coulomb repulsion recently introduced by Brandt and Giesekus. We point out that the exact ground state can be regarded as a resonating-valence-bond state, and argue that the state may exhibit superconductivity. The existence of a phase with singlet-pair ordering is demonstrated in a simple model on a tree.

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Whether *repulsive* Coulomb interactions between itinerant electrons can lead to a superconductivity has been an interesting unsolved problem [1]. Numerical works on the standard single-band Hubbard model seem to indicate the absence of superconducting phases, but, considering the remarkable "nonuniversal" behavior of the Hubbard model, it is still possible that a class of models with specific band structure and filling factor exhibit superconductivity. The aim of the present Letter is to discuss a class of solvable Hubbard models, which might provide the simplest examples in a "universality class" of repulsive Hubbard models which exhibit superconductivity.

Recently Brandt and Giesekus [2] introduced an extended Hubbard model with infinitely large on-site Coulomb repulsion on the decorated hypercubic lattice. They were able to construct exact ground states for certain filling factors. Mielke [3] showed that the construction can be generalized to Hubbard models on a general class of line graphs. In these works, it was argued that the exact ground states have paramagnetic character. See [4] for Strack's different extensions.

In the present Letter, we further generalize the Brandt-Giesekus model to a class of lattices with certain cell structure. We then point out that the exact ground states can be regarded as resonating-valence-bond (RVB) states [5] with a certain sign rule characteristic of a system governed by electron (or hole) motion [6]. The standard procedure in valence-bond states allows one to express various ground state expectation values as that in a stochastic geometric system of random loops (with, however, not necessarily positive statistical weights). We argue that a possible percolation in the random loop system may correspond to a superconductivity in the original electron model. To make this idea more concrete, we study the simplest version of the model on a tree, and show that the ground state develops a singlet-pair ordering.

We define the model in its most generalized form [7]. Consider a finite lattice Λ, and assume that it can be written as $\Lambda = \cup_{i=1}^{N_c} C_i$, where each C_i is called a *cell*. A site $x \in \Lambda$ may belong to several different cells (Fig. 1). In a cell C_i, we assign a constant $\lambda_x^{(i)} > 0$ to each $x \in C_i$. (When x belongs to more than one cell, $\lambda_x^{(i)}$ can be chosen independently in each cell.) We define the hopping Hamiltonian within the cell as

$$H(C_i) = -\sum_{x,y\in C_i,\sigma=\uparrow,\downarrow} t_{xy}^{(i)} c_{x\sigma}^{\dagger} c_{y\sigma} + \sum_{x\in C_i} t_{xx}^{(i)}, \qquad (1)$$

where $t_{xy}^{(i)} = \lambda_x^{(i)}\lambda_y^{(i)}$ if $x \neq y$, and $t_{xx}^{(i)} = 2(\lambda_x^{(i)})^2$. Here $c_{x\sigma}^{\dagger}$ and $c_{x\sigma}$ are the creation and annihilation operators, respectively, of an electron at site x with spin $\sigma = \uparrow, \downarrow$. The electron number operators are defined as $n_{x\sigma} = c_{x\sigma}^{\dagger} c_{x\sigma}$ and $n_x = n_{x\uparrow} + n_{x\downarrow}$. The full Hamiltonian of the model is

$$H = P \sum_{i=1}^{N_c} H(C_i)\, P, \qquad (2)$$

where the Gutzwiller projection operator $P = \prod_{x\in\Lambda}(1 - n_{x\uparrow}n_{x\downarrow})$ exactly takes into account the effect of the infinitely large on-site Coulomb repulsion.

The above class of models reduces to that considered by Mielke [3] when each site belongs to exactly two cells, two distinct cells share at most one site in common, and all $\lambda_x^{(i)}$ are identical. It reduces to the original class of Brandt and Giesekus if one further restricts the lattice to the decorated hypercubic lattice (the line graph of the hypercubic lattice). It is expected that the inclusion of model parameters and various lattice structures increases the chance of finding nontrivial physics from the solvable

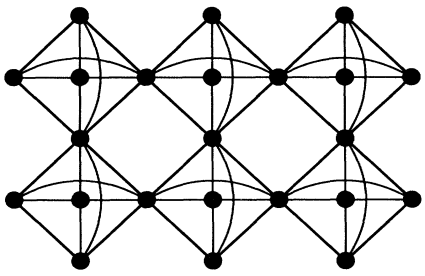

FIG. 1. A typical lattice in two dimensions. Each cell contains 5 sites. We get an exact ground state when the electron filling factor is equal to 1/3.

models. In particular, allowing the neighboring cells to share more than one site in common enhances the tendency of the condensation of singlet electron pairs (valence bonds), as can be seen from the geometric representation (7) that we develop.

Following Brandt and Giesekus [2], we use the operator identities $-Pc^\dagger_{x\sigma}c_{y\sigma}P = c_{y\sigma}Pc^\dagger_{x\sigma}$ for $x \neq y$, and $P(1-n_x)P = c_{x\sigma}Pc^\dagger_{x\sigma}$ to rewrite the Hamiltonian (2) as

$$H = \sum_{i=1}^{N_c} \sum_{\sigma=\uparrow,\downarrow} a_{i\sigma} P a^\dagger_{i\sigma}, \tag{3}$$

where $a_{i\sigma} = \sum_{x\in C_i} \lambda^{(i)}_x c_{x\sigma}$. Let us define

$$|\Phi_{GS}\rangle = P \prod_{i=1}^{N_c} \prod_{\sigma=\uparrow,\downarrow} a^\dagger_{i\sigma} |\Phi_0\rangle, \tag{4}$$

where $|\Phi_0\rangle$ is the vacuum state. Using $(Pa^\dagger_{i\sigma})^2 = 0$, we find that the state (4) satisfies $H|\Phi_{GS}\rangle = 0$. Since the Hamiltonian H is positive semidefinite [from the representation (3)], this shows that $|\Phi_{GS}\rangle$ is an exact ground state of the model, provided that it is nonvanishing. By using the overlap formula (6), we can prove [8] that the state (4) is nonvanishing for a general class of models with free boundary conditions [9]. See [2, 3, 8] for other criteria for (4) to be nonvanishing.

Brandt and Giesekus conjectured that, in their model, (4) is the unique ground state in the subspace with the electron number $\sum_{x\in\Lambda} n_x$ fixed to $2N_c$. We believe the same for the present generalization [10], but we have no proof.

Note that the ground state (4) can be written as

$$|\Phi_{GS}\rangle = P \prod_{i=1}^{N_c} \sum_{x>y\in C_i} \lambda_x \lambda_y b^\dagger_{xy} |\Phi_0\rangle, \tag{5}$$

where $b^\dagger_{xy} = c^\dagger_{x\uparrow}c^\dagger_{y\downarrow} + c^\dagger_{y\uparrow}c^\dagger_{x\downarrow}$ is the creation operator of the "valence bond" (singlet pair) on sites x and y. It is remarkable that (5) has the form of the so-called RVB state [5], in the sense that it is a superposition of various states which are products of singlet pairs [11]. Note that all the basis states have nonnegative coefficients in the state (5). This is in contrast with the "standard" RVB states found as the ground states of Heisenberg antiferromagnets on bipartite lattices, where the coefficients have oscillating signs [12] in order to satisfy the Marshall-Lieb-Mattis sign rule [13]. In [6], it was argued from a general consideration of a large-n version of the t-J model that the natural relative sign for the ground state in a system governed by electron (or hole) motion [14] should be as in the above (5).

By identifying the ground state (4) as an RVB state (5), we can make use of the standard random loop representation technique [15] for valence-bond states. Let the valence-bond configuration V be a set of N_c bonds (i.e., pairs of sites) constructed by choosing one bond from each cell in a way that any pair of bonds in V have no sites in common. For valence-bond configurations V and V', we have [6, 8]

$$\langle\Phi_0| \prod_{\{x,y\}\in V} b_{xy} \prod_{\{u,v\}\in V'} b^\dagger_{uv} |\Phi_0\rangle = \prod_{i=1}^{n(V\cup V')} 2(-1)^{|\ell_i|/2-1}, \tag{6}$$

provided that the graph $V \cup V'$ consists only of closed loops. Otherwise the quantity is vanishing. We have decomposed the graph as $V \cup V' = \cup_{i=1}^{n(V\cup V')} \ell_i$ where each ℓ_i is a connected closed loop and $|\ell_i|$ denotes the number of bonds in ℓ_i. By using (5) and (6) we find that the overlap of the ground state with itself can be represented as

$$\langle\Phi_{GS}|\Phi_{GS}\rangle = \sum_{V,V'} \lambda(V)\lambda(V') \prod_{i=1}^{n(V\cup V')} 2(-1)^{|\ell_i|/2-1}, \tag{7}$$

where the sum is taken over valence-bond configurations V and V' with the property that $V \cup V'$ consists only of closed loops. These loops are denoted as ℓ_i with $i = 1, 2, \ldots, n(V \cup V')$. We have set $\lambda(V) = \prod_{\{x,y\}\in V} \lambda_{xy}$.

The right-hand side of (7) defines a stochastic geometric system of random loops. Although the probabilistic interpretation is not precise because of the oscillating sign in the statistical weights, this analogy helps us to develop pictures about the behavior of the system based on "classical" intuitions. A typical condensation phenomenon one expects in a system of random loops is percolation, which is characterized by the appearance of an infinitely large loop. By using (6), one gets the representation

$$\langle\Phi_{GS}| b_{xy} b^\dagger_{uv} |\Phi_{GS}\rangle = \sum_{V,V'} \lambda(V)\lambda(V') \prod_{i=1}^{n(V\cup V'\cup\{x,y\}\cup\{u,v\})} 2(-1)^{|\ell_i|/2-1}, \tag{8}$$

where V and V' are summed over the valence-bond configurations with the property that $V\cup V'\cup\{x,y\}\cup\{u,v\}$ consists only of closed loops, which are again denoted as ℓ_i. When neither $\{x,y\}$ nor $\{u,v\}$ is contained in a single cell, the graph $V\cup V'\cup\{x,y\}\cup\{u,v\}$ has a connected loop which contains both the bonds $\{x,y\}$ and $\{u,v\}$. This observation suggests that the percolation in the random loop system manifests itself as a long range order in the singlet-pair correlation function $\langle b_{xy} b^\dagger_{uv}\rangle$, where we keep x and y (respectively, u and v) close to each other, and separate two pairs by a large distance. The existence of such an off-diagonal order is usually expected to indicate a superconductivity [16].

In order to check the above idea in a concrete situation, we shall consider a model on a tree. Although it is possible to consider many variants of tree models [8],

we discuss here the simplest one. The tree is constructed recursively as follows. The cell in this model consists of p sites with $p \geq 5$. We call one of them the origin of the cell, and denote it as o. We define the hopping Hamiltonian (1) within the cell by setting $\lambda_o = \lambda > 0$ and $\lambda_x = 1$ for $x \neq o$. The first order tree consists of a single cell. The origin of the cell is called the origin of the tree and the remaining sites are called the boundary of the tree. The nth order tree is constructed from a cell and $(p-1)$ copies of the $(n-1)$th order tree. We identify each site $x \neq o$ of the cell with the origin of an $(n-1)$th order tree. The boundary B_n of the resulting tree is the union of the boundaries of the $(n-1)$th order trees, and the origin (again denoted as o) of the tree is that of the cell (Fig. 2).

We consider the Hubbard model on the nth order tree with the Hamiltonian (3). The state (4) is the exact ground state when the electron number is equal to $2N_c$, where N_c is the total number of cells. In order to test for the existence of electron pairing in the ground state (4), we shall look at the off-diagonal correlation function between a singlet pair including the origin of the tree and the (sum of) singlet pairs at the boundary of the tree. It is given by $S_n = \langle \Phi_{GS}| d_\uparrow d_\downarrow b^\dagger_{ox} |\Phi_{GS}\rangle \,/\, \langle \Phi_{GS}|\Phi_{GS}\rangle$, where x is a site neighboring to the origin o of the tree (Fig. 2), and $d_\sigma = \sum_{u \in B_n} c_{u\sigma}$.

Let X_n be the quantity defined by the right-hand side of (7), but with the sum taken over V and V' on the nth order tree such that the graph $V \cup V'$ consists of usual closed loops and an open path connecting a boundary site and the origin. Similarly Y_n and Z_n are the sums over V and V' where $V \cup V'$ has only closed loops, but the origin is empty in the former and is occupied in the latter. A simple calculation shows that $S_n = (p-2)(p-3)(X_{n-1})^2 Y_{n-1}(Y_{n-1} + Z_{n-1})^{p-4}/(Y_n + Z_n)$. It is also easy to verify that these quantities satisfy the following recursion relations:

$$\begin{aligned} X_{n+1} &= \lambda(p-1)(p-2) X_n Y_n (Y_n + Z_n)^{p-3}, \\ Y_{n+1} &= (p-1)(p-2)(Y_n)^2 (Y_n + Z_n)^{p-3}, \\ Z_{n+1} &= 2\lambda^2 (p-1) Y_n (Y_n + Z_n)^{p-2}. \end{aligned} \tag{9}$$

In terms of the normalized quantities $x_n = X_n/Y_n$ and $z_n = Z_n/Y_n$, the recursion relation (9) becomes simple as $x_{n+1} = \lambda x_n$ and $z_{n+1} = \{2\lambda^2/(p-2)\}(1+z_n)$. The map for x_n is trivial, and gives $x_n = \lambda^n x_0$. The asymptotic behavior of z_n as $n \to \infty$ is given by $z_n \to z^* = \{1 - 2\lambda^2/(p-2)\}^{-1}$ for $\lambda \leq \sqrt{(p-2)/2}$, and $z_n \sim \{2\lambda^2/(p-2)\}^n$ for $\lambda > \sqrt{(p-2)/2}$. By noting that the singlet-pair correlation function S_n can be expressed in terms of the normalized quantities as $S_{n+1} = (p-2)(p-3)(x_n)^2 (z_n+1)^{p-4}/\{(p-1)(p-2)(z_n+1)^{p-3} + 2\lambda^2(p-1)(z_n+1)^{p-2}\}$, its asymptotic behavior as $n \to \infty$ is obtained as

$$S_n \sim \begin{cases} \lambda^{2n} & \text{for } 0 < \lambda \leq \sqrt{(p-2)/2}, \\ \left(\frac{p-2}{2\lambda}\right)^{2n} & \text{for } \lambda > \sqrt{(p-2)/2}. \end{cases} \tag{10}$$

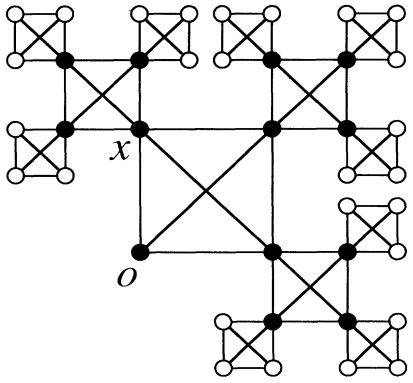

FIG. 2. The third order tree with $p = 4$. Open circles form the boundary B_n.

We find that the correlation grows exponentially in the parameter region $1 < \lambda < (p-2)/2$, which may be interpreted as a sign of the formation of a long range singlet-pair ordering [17], i.e., a superconductivity.

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[8] H. Tasaki (to be published).
[9] It is obvious that, for the state (4) to be nonvanishing, one must have sufficiently many sites so that one can assign two sites with each cell.
[10] Brandt and Giesekus [2] briefly discuss general cases with the electron number not less than $2N_c$ as well, but we shall here concentrate on the case where it is equal to $2N_c$.
[11] Reflecting the RVB character, a naive mean-field theory should predict that the ground state (4) exhibits a superconductivity. This may be regarded as a concrete realization of the scenario proposed by Anderson [1].
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dominated RVB) states. These two types of RVB states can be clearly distinguished with each other from the sign rules and symmetry [6]. Before [6], a transition between the two types of RVB states was observed numerically in K. Takano and K. Sano, Phys. Rev. B **39**, 7367 (1989).

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[17] Even when S_n grows exponentially in n, each correlation function $\langle c_{u\uparrow} c_{v\downarrow} b^{\dagger}_{ox} \rangle$ (with $u, v \in B_n$) decays exponentially in n. This fact might sound as a negative sign for the occurrence of an order. But we believe that an exponential growth in center-to-boundary correlation (like S_n) in a tree model corresponds to an order in local correlations in models on standard lattices. This is precisely the case in, say, the ferromagnetic Ising model. See, for example, C. J. Thompson, J. Stat. Phys. **27**, 441 (1982).