New Exactly Solvable Model of Strongly Correlated Electrons Motivated by High-T_c Superconductivity

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We present a new model describing strongly correlated electrons on a general d-dimensional lattice. It is an extended Hubbard model and it contains the t-J model as a special case. The model naturally describes local electron pairs, which can move coherently at arbitrary momentum. By using an η-pairing mechanism we can construct eigenstates of the Hamiltonian with off-diagonal long-range order. In the attractive case the exact ground state is superconducting in any number of dimensions. On a one-dimensional lattice, the model is exactly solvable by Bethe ansatz.

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The study of strongly correlated electrons on a lattice is an important tool in theoretical condensed-matter physics in general, and in the study of high-T_c superconductivity in particular. Two well-studied models are the Hubbard model and the t-J model. On a one-dimensional lattice these models are both exactly solvable by Bethe ansatz. In this Letter we propose a new model, which is again solvable in one dimension, and which combines and extends some of the interesting features of the Hubbard model and the t-J model.

Electrons on a lattice are described by operators $c_{j,\sigma}$, $j=1,\ldots,L$, $\sigma=\uparrow,\downarrow$, where L is the total number of lattice sites. These are canonical Fermi operators with anticommutation relations given by $\{c^\dagger_{i,\sigma},c_{j,\tau}\}=\delta_{i,j}\delta_{\sigma,\tau}$. The state $|0\rangle$ (the Fock vacuum) satisfies $c_{i,\sigma}|0\rangle=0$. At a given lattice site i there are four possible electronic states:

$$|0\rangle,\quad |\uparrow\rangle_i=c^\dagger_{i,\uparrow}|0\rangle,$$
$$|\downarrow\rangle_i=c^\dagger_{i,\downarrow}|0\rangle,\quad |\uparrow\downarrow\rangle_i=c^\dagger_{i,\downarrow}c^\dagger_{i,\uparrow}|0\rangle. \tag{1}$$

By $n_{i,\sigma}=c^\dagger_{i,\sigma}c_{i,\sigma}$ we denote the number operator for electrons with spin σ on site i and we write $n_i=n_{i,\uparrow}+n_{i,\downarrow}$. The spin operators $S=\sum_{j=1}^L S_j$, $S^\dagger$, and S^z,

$$S_j=c^\dagger_{j,\uparrow}c_{j,\downarrow},\quad S^\dagger_j=c^\dagger_{j,\downarrow}c_{j,\uparrow},\quad S^z_j=\tfrac{1}{2}(n_{j,\uparrow}-n_{j,\downarrow}), \tag{2}$$

form an SU(2) algebra and they commute with the Hamiltonians that we consider below. (We shall always give local expressions $\mathcal{O}_j$ for symmetry generators, implying that the global ones are obtained as $\mathcal{O}=\sum_{j=1}^L\mathcal{O}_j$.)

The Hubbard model Hamiltonian can be written as

$$H^{\text{Hubbard}}=-\sum_{\langle jk\rangle}\sum_{\sigma=\uparrow,\downarrow}(c^\dagger_{j,\sigma}c_{k,\sigma}+c^\dagger_{k,\sigma}c_{j,\sigma})+U\sum_{j=1}^L(n_{j,\uparrow}-\tfrac{1}{2})(n_{j,\downarrow}-\tfrac{1}{2}), \tag{3}$$

where the first summation runs over all nearest-neighbor pairs $\langle jk\rangle$. It contains kinetic (hopping) terms for the electrons and an on-site interaction term for electron pairs. An interesting feature (on a bipartite periodic lattice) is the so-called η-pairing symmetry [1,2], which involves operators η_H, $\eta^\dagger_H$, and η^z_H which form another SU(2) algebra, and which commute with the Hamiltonian (3). Using this symmetry one can, starting from an eigenstate $|\psi\rangle$ of the Hamiltonian, create a new eigenstate $\eta^\dagger_H|\psi\rangle$, which contains an additional local electron pair of momentum π. The spin SU(2) algebra (2) and the η-pairing SU(2) algebras together form an SO(4) symmetry algebra. In one dimension, the Hubbard model is solvable by Bethe ansatz [3].

In the t-J model, there is a kinematical constraint which forbids the occurrence of two electrons on the same lattice site. On this restricted Hilbert space the t-J Hamiltonian (with $t=1$, $J=2$) acts as $H^{t\text{-}J}=-\sum_{\langle jk\rangle}H^{t\text{-}J}_{j,k}$, with

$$H^{t\text{-}J}_{j,k}=\sum_{\sigma=\uparrow,\downarrow}(Q^\dagger_{j,\sigma}Q_{k,\sigma}+Q^\dagger_{k,\sigma}Q_{j,\sigma})-2[S^z_jS^z_k+\tfrac{1}{2}(S^\dagger_jS_k+S_jS^\dagger_k)-\tfrac{1}{2}(1-n_j-n_k)-\tfrac{1}{4}n_jn_k], \tag{4}$$

where we defined

$$Q_{j,\uparrow}=(1-n_{j,\downarrow})c_{j,\uparrow},\quad Q_{j,\downarrow}=(1-n_{j,\uparrow})c_{j,\downarrow}, \tag{5}$$

and the operators S^z_j, S_j, and $S^\dagger_j$ are as in (2). The t-J model (4) is supersymmetric and the spin SU(2) symmetry algebra gets enlarged to the superalgebra SU(1|2) [4,5] (see [6] for the description and classification of the classical Lie superalgebras). The generators of this symmetry algebra are S, $S^\dagger$, S^z, $Q_\uparrow$, $Q^\dagger_\uparrow$, $Q_\downarrow$, $Q^\dagger_\downarrow$, and $T=2L-\sum_{j=1}^L n_j$. In one dimension the supersymmetric t-J model (4) is exactly solvable by Bethe ansatz [7-9].

Before we present the Hamiltonian of the new model, we give some motivation, which is based on what we know about the materials that exhibit high-T_c superconductivity. It has been found that the electrons in these materials form "Cooper pairs," which are spin singlets, and that these pairs are much smaller than in the traditional superconductors. As a limiting case one can consider models which have electron pairs of size zero, i.e., pairs that are localized on single lattice sites. We will call such localized electron pairs *localons*.

In the t-J model localons are ruled out by the kinematical constraint on the space of states, and in the Hubbard model only local pairs of momentum π exist. Below we shall see that in our new model localons can move coherently with arbitrary momentum. Apart from these local pairs, the new model may also have bound states that are finite-size electron pairs.

Let us now present the Hamiltonian of the new model on a general d-dimensional lattice. We write it as

$$H=H^0+U\sum_{j=1}^{L}(n_{j,\uparrow}-\tfrac{1}{2})(n_{j,\downarrow}-\tfrac{1}{2})+\mu\sum_{j=1}^{L}n_j+h\sum_{j=1}^{L}(n_{j,\uparrow}-n_{j,\downarrow}), \quad (6)$$

where H^0 is given by

$$H^0=-\sum_{\langle jk\rangle}H^0_{j,k}, \quad (7)$$

$\langle j,k\rangle$ are nearest neighbors, with

$$\begin{aligned}H^0_{j,k}=&c^\dagger_{k,\uparrow}c_{j,\uparrow}(1-n_{j,\downarrow}-n_{k,\downarrow})+c^\dagger_{j,\uparrow}c_{k,\uparrow}(1-n_{j,\downarrow}-n_{k,\downarrow})+c^\dagger_{k,\downarrow}c_{j,\downarrow}(1-n_{j,\uparrow}-n_{k,\uparrow})+c^\dagger_{j,\downarrow}c_{k,\downarrow}(1-n_{j,\uparrow}-n_{k,\uparrow})\\&+\tfrac{1}{2}(n_j-1)(n_k-1)+c^\dagger_{j,\uparrow}c^\dagger_{j,\downarrow}c_{k,\downarrow}c_{k,\uparrow}+c_{j,\downarrow}c_{j,\uparrow}c^\dagger_{k,\uparrow}c^\dagger_{k,\downarrow}-\tfrac{1}{2}(n_{j,\uparrow}-n_{j,\downarrow})(n_{k,\uparrow}-n_{k,\downarrow})\\&-c^\dagger_{j,\downarrow}c_{j,\uparrow}c^\dagger_{k,\uparrow}c_{k,\downarrow}-c^\dagger_{j,\uparrow}c_{j,\downarrow}c^\dagger_{k,\downarrow}c_{k,\uparrow}+(n_{j,\uparrow}-\tfrac{1}{2})(n_{j,\downarrow}-\tfrac{1}{2})+(n_{k,\uparrow}-\tfrac{1}{2})(n_{k,\downarrow}-\tfrac{1}{2}).\end{aligned} \quad (8)$$

This Hamiltonian contains kinetic terms and interaction terms that combine those of the Hubbard and of the t-J model. The second term in (6) is the on-site Hubbard interaction term (notice that it also gets a contribution from H^0). The third and fourth terms in (6) introduce a chemical potential μ and a magnetic field h. Roughly speaking, the new model can be viewed as a modified Hubbard model with additional nearest-neighbor interactions similar to those in the t-J model.

The Hamiltonian H^0 is invariant under spin-reflection $c_{j,\uparrow}\leftrightarrow c_{j,\downarrow}$ and under particle-hole replacement $c^\dagger_{j,\sigma}\leftrightarrow c_{j,\sigma}$. In addition to the spin SU(2) generators (2), the following operators commute with H^0.

η-pairing SU(2).—The generators are η, $\eta^\dagger$, and η^z:

$$\eta_j=c_{j,\uparrow}c_{j,\downarrow},\quad \eta^\dagger_j=c^\dagger_{j,\downarrow}c^\dagger_{j,\uparrow},\quad \eta^z_j=-\tfrac{1}{2}n_j+\tfrac{1}{2}. \quad (9)$$

Together with the spin SU(2) algebra (2), this gives an SO(4) algebra which is similar to the one for the Hubbard model. This symmetry makes it possible to generalize the η-pairing mechanism, which was developed for the Hubbard model in [2], to the new model.

Supersymmetries.—There are eight supersymmetries in total: $Q_\uparrow$, $Q^\dagger_\uparrow$, $Q_\downarrow$, and $Q^\dagger_\downarrow$ given in (5) and the operators $\tilde{Q}_\sigma$ and $\tilde{Q}^\dagger_\sigma$:

$$\tilde{Q}_{j,\uparrow}=n_{j,\downarrow}c_{j,\uparrow},\quad \tilde{Q}_{j,\downarrow}=n_{j,\uparrow}c_{j,\downarrow}. \quad (10)$$

These generators, together with the operator $\sum_{j=1}^{L}1$ (which is constant and equal to L), form the superalgebra SU(2|2). [Like SU(4), this algebra has fifteen generators, eight of which are fermionic. In the fundamental representation, the generators can be represented as 4×4 supermatrices with vanishing supertrace [6].]

The symmetries of the Hamiltonian H^0 can be made manifest as follows. We first add one more generator to the symmetry algebra, which is

$$X=\sum_{j=1}^{L}X_j,\quad X_j=(n_{j,\uparrow}-\tfrac{1}{2})(n_{j,\downarrow}-\tfrac{1}{2}),\quad [H^0,X]=0. \quad (11)$$

This extends the superalgebra SU(2|2) to U(2|2). We denote the generators of this algebra by J_α, where $\alpha=1,2,\ldots,16$. We now introduce an invariant, nondegenerate two-index tensor, denoted by $K^{\alpha\beta}$, which is the inverse of $K_{\alpha\beta}=\mathrm{str}(J_\alpha J_\beta)$ (str denotes supertrace), where the J_α are 4×4 supermatrices in the fundamental representation. Using this, we can cast $H^0_{j,k}$ in a group-theoretical form, as follows:

$$H^0_{j,k}=\sum_{\alpha,\beta=1}^{16}K^{\alpha\beta}J_{j,\alpha}J_{k,\beta} \quad (12)$$

$$\begin{aligned}&=\sum_{\sigma=\uparrow,\downarrow}(Q^\dagger_{j,\sigma}Q_{k,\sigma}+Q^\dagger_{k,\sigma}Q_{j,\sigma}-\tilde{Q}^\dagger_{j,\sigma}\tilde{Q}_{k,\sigma}-\tilde{Q}^\dagger_{k,\sigma}\tilde{Q}_{j,\sigma})\\&\quad+(2\eta^z_j\eta^z_k+\eta^\dagger_j\eta_k+\eta_j\eta^\dagger_k)\\&\quad-(2S^z_jS^z_k+S^\dagger_jS_k+S_jS^\dagger_k)+X_j+X_k.\end{aligned} \quad (13)$$

It is easily checked that this expression agrees with the formula for $H^0_{j,k}$ in (8). The expression (12) immediately makes it clear that H^0 commutes with all sixteen generators of U(2|2).

We would like to stress that the appearance of the algebra U(2|2) in the model is not too surprising: On each lattice site there are four electronic states (1), two of which are fermionic. The supergroup U(2|2) is the group of all unitary rotations of these four states into one another. Our Hamiltonian H^0 has been chosen such that it commutes with the entire algebra U(2|2) and is therefore very natural. The analogous construction for U(1|2) leads to the t-J Hamiltonian (4), and for U(2) it leads to the spin-$\tfrac{1}{2}$ XXX Heisenberg model.

The spectrum of the Hamiltonian H^0 is symmetric around zero. This follows from the discrete symmetry $c^\dagger_{j,\downarrow}\leftrightarrow c_{j,\downarrow}$, for which $H^0\leftrightarrow -H^0$.

There is a further aspect of H^0 that deserves to be mentioned: The terms $H^0_{j,k}$ act as graded permutations of the electron states (1) at sites j and k. By "graded" we mean that there is an extra minus sign if the two states that are permuted are both (fermionic) single-electron states. For example,

$$H^0_{j,k}c^\dagger_{j,\uparrow}|0\rangle = c^\dagger_{k,\uparrow}|0\rangle, \quad H^0_{j,k}c^\dagger_{j,\uparrow}c^\dagger_{k,\downarrow}|0\rangle = -c^\dagger_{j,\downarrow}c^\dagger_{k,\uparrow}|0\rangle, \ldots . \tag{14}$$

In this respect, the new model generalizes the spin-$\frac{1}{2}$ XXX model and the t-J model (4). The nearest-neighbor Hamiltonians of these models have a similar interpretation as graded permutations of the basic states, which are $\{|\uparrow\rangle,|\downarrow\rangle\}$ for the spin-$\frac{1}{2}$ XXX model and $\{|0\rangle,|\uparrow\rangle,|\downarrow\rangle\}$ for the t-J model. Lattice Hamiltonians that act like (graded) permutations were first considered by Sutherland in [8].

We define the number operators $N_\uparrow, N_\downarrow$ (the number of single electrons with given spin) and N_l (the number of localons) by

$$N_\uparrow + N_l = \sum_{j=1}^{L} n_{j,\uparrow}, \quad N_\downarrow + N_l = \sum_{j=1}^{L} n_{j,\downarrow}, \quad N_l = \sum_{j=1}^{L} n_{j,\uparrow}n_{j,\downarrow}, \tag{15}$$

and we write $N_e = N_\uparrow + N_\downarrow$ for the total number of single electrons. The fact that H^0 is a permutation makes it clear that these number operators commute with H^0, so that H^0 can be diagonalized within a sector with given numbers $N_\uparrow$, $N_\downarrow$, and N_l. This implies that the terms proportional to U, μ, and h in (6), which break the symmetry U(2|2), will not affect the solvability of the model in one dimension.

In the sectors without localons H^0 reduces to the t-J Hamiltonian (4). (This is clear from the fact that they both act as permutations.) The new model reduces to the spin-$\frac{1}{2}$ XXX model in the sector with only vacancies and localons, and similarly in the (half-filled) sector with one single electron on each site.

Let us now briefly discuss some physical aspects of the new model. We first remark that we can always (for general lattices in an arbitrary number of dimensions) construct a number of exact eigenstates of the Hamiltonian which show off-diagonal long-range order (ODLRO), which is characteristic for superconductivity [10]. For this we follow the construction which was developed for the Hubbard model by Yang in [2]. The state $\Psi_N = (\eta^\dagger)^N|0\rangle$ is an eigenstate of the Hamiltonian with energy $E = 2\mu N + UL/4 - M$, where M is the total number of nearest-neighbor links $\langle jk\rangle$ in the lattice. Following [2], we compute the following off-diagonal matrix element $(k\neq l)$ of the reduced density matrix ρ_2:

$$\langle (k,\downarrow)(k,\uparrow)|\rho_2|(l,\uparrow)(l,\downarrow)\rangle = \frac{\langle 0|\eta^N c^\dagger_{k,\downarrow}c^\dagger_{k,\uparrow}c_{l,\uparrow}c_{l,\downarrow}(\eta^\dagger)^N|0\rangle}{\langle 0|\eta^N(\eta^\dagger)^N|0\rangle} = \frac{N(L-N)}{L(L-1)} . \tag{16}$$

The fact that this off-diagonal matrix element is constant for large distances $|j-k|$ establishes the property of ODLRO for the states Ψ_N.

An important observation is that for the attractive case $(U<0)$ with zero magnetic field $(h=0)$, the ground state in the sector with an even number $2N$ of electrons is precisely the state $\Psi_N = (\eta^\dagger)^N|0\rangle$. It can be rigorously shown that within each of these sectors (positive density corresponds to negative μ) this ground state is unique. We may thus conclude that in the attractive case our new model exhibits superconductivity.

The local electron pairs that participate in the η pairing have momentum zero. However, the model also admits localons that move with arbitrary momentum. This follows from the fact that $H^0_{j,k}$ acts as a permutation of the electronic states (1) on neighboring sites: Because of this localons cannot decay and move coherently. On a d-dimensional square lattice (with lattice spacing a) the wave function $\sum_{\mathbf{x}}\exp(i\mathbf{x}\cdot\mathbf{k})c^\dagger_{\mathbf{x},\uparrow}c^\dagger_{\mathbf{x},\downarrow}|0\rangle$, which describes a single localon of momentum $\mathbf{k}$ over the bare vacuum, is an exact eigenfunction of the Hamiltonian (6) of energy

$$E = 2d - 2\sum_{m=1}^{d}\cos(k_m a) + UL/4 + 2\mu - M . \tag{17}$$

Multilocalon wave functions, as well as wave functions with single electrons, exist but cannot easily be written down for higher-dimensional lattices. However, in one dimension the model is exactly solvable by Bethe ansatz (BA), and we can obtain explicit expressions for general eigenstates of the Hamiltonian. We think that it is worthwhile to study this exact solution, and that this will lead to a better understanding of the higher-dimensional model as well.

We will here briefly summarize the results of the exact solution in one dimension; the details are deferred to a separate publication [11]. The exact solution starts from the observation that the Hamiltonian is a graded permutation (14) of four states, of which two are fermionic and two are bosonic. The BA analysis for Hamiltonians which are graded permutations was first considered by Sutherland in [8]; see also [12]. The method of solution is the algebraic version of the "nested Bethe ansatz" [13] (for an introduction to the algebraic BA, see [14]). Each step of the nesting involves the introduction of a set of spectral parameters, which are in our case λ_j, $\lambda^{(1)}_k$, and $\lambda^{(2)}_l$, where $j=1,\ldots,(N_e+N_l)$, $k=1,\ldots,N_e$, and $l=1,\ldots,N_\downarrow$.

For each choice of a set of rapidities we can construct an eigenstate of the Hamiltonian H^0 in the sector specified by N_l, N_e, and $N_\downarrow$, with energy E^0 given by

$$E^0 = \sum_{j=1}^{N_e+N_l} 1/(\lambda_j^2 + \tfrac{1}{4}) - L . \tag{18}$$

The boundary conditions for these eigenstates lead to the following set of Bethe equations for the rapidities λ_j, $\lambda^{(1)}_k$, and $\lambda^{(2)}_l$:

$$\left(\frac{\lambda_j - i/2}{\lambda_j + i/2}\right)^L = \prod_{\substack{j'=1 \\ j' \neq j}}^{N_e+N_l} \frac{\lambda_j - \lambda_{j'} - i}{\lambda_j - \lambda_{j'} + i} \prod_{k'=1}^{N_e} \frac{\lambda_{k'}^{(1)} - \lambda_j - i/2}{\lambda_{k'}^{(1)} - \lambda_j + i/2},$$

$$\prod_{j'=1}^{N_e+N_l} \frac{\lambda_k^{(1)} - \lambda_{j'} + i/2}{\lambda_k^{(1)} - \lambda_{j'} - i/2} = \prod_{l'=1}^{N_\downarrow} \frac{\lambda_k^{(1)} - \lambda_{l'}^{(2)} + i/2}{\lambda_k^{(1)} - \lambda_{l'}^{(2)} - i/2}, \qquad (19)$$

$$\prod_{\substack{l'=1 \\ l' \neq l}}^{N_\downarrow} \frac{\lambda_{l'}^{(2)} - \lambda_l^{(2)} + i}{\lambda_{l'}^{(2)} - \lambda_l^{(2)} - i} = \prod_{k'=1}^{N_e} \frac{\lambda_{k'}^{(1)} - \lambda_l^{(2)} + i/2}{\lambda_{k'}^{(1)} - \lambda_l^{(2)} - i/2}.$$

These equations, together with the expression (18) for the energy, guarantee that we shall be able to describe explicitly the ground state of our model for arbitrary density of electrons, coupling constant U, and magnetic field h [11].

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