Model of Fermions with Correlated Hopping (Integrable Cases)

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We present a new model describing strongly correlated electrons on a lattice. The model naturally describes the nearest-neighbor hopping of electrons and local electron pairs and the interaction between them. It is an extended Hubbard model exactly solvable in one dimension for some special values of the coupling constants. The Bethe ansatz equation are obtained and a ground state is discussed.

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The discovery of the phenomena of high T_c superconductivity stimulates the construction and investigation of new integrable models in theoretical condensed matter physics. The one-dimensional integrable model of fermions interacting via the interorbital exchange interaction has been recently proposed by Schlottmann [1]. In [2] the authors focus attention on the superconducting model of strongly correlated electrons which is exactly solvable by the Bethe ansatz in one dimension.

Among models of correlated electrons the Hubbard and t-J ones play an important role in the study of the microscopic mechanism for superconductivity in the electronic subsystems of transition metal oxide compounds. The crucial step for our present understanding of the one-dimensional Hubbard model was made by Lieb and Wu [3] who have solved it exactly using the Bethe ansatz. The one-dimensional t-J model is integrable for a specific value of the ratio $t/2J = \pm 1$ [4]. This specific point corresponds to supersymmetric invariance of the model Hamiltonian [5–7].

In this Letter we propose a new integrable narrow-band model of strongly correlated electrons. The model describes the chain of itinerant electrons with the Hamiltonian that includes the correlated hopping of electrons between nearest-neighbor sites and the repulsion (attraction) of two electrons on the same site. The model also admits existence of local electron pairs, which can move along chain interacting with itinerant electrons. Roughly speaking this model can be viewed as a modified Hubbard model with correlated nearest-neighbor hopping.

The electron states on a lattice are conveniently determined by the use of the Hubbard operators X_i^{ab} which describe all possible configurations of electrons at given lattice site $i|a\rangle = X_i^{a0}|0\rangle\,(a = 0,\uparrow,\downarrow,2)$, where $|0\rangle$ denotes the Fock vacuum, $i = 1,2,\ldots,N_a$, N_a is the total number of lattice sites. The Hubbard operators form a basis of superalgebra SU(2|2). The algebra SU(2|2) has a total of 16 generators, 8 of which are fermionic and bosonic, respectively. The structure of the composition rules is

$$[X_i^{ab}, X_j^{cd}]_{\pm} = \delta_{ij}(\delta^{bc}X_i^{ad} \pm \delta^{ad}X_i^{cb}), \tag{1}$$

where $[,]_{\pm}$ denotes a graded commutator, $[A,B] = AB - (-1)^{\epsilon_a\epsilon_b}BA$, here ϵ_a and ϵ_b are Grassmann parities of the operators A and B, respectively (i.e., $\epsilon = 1$ for the fermionic operators and $\epsilon = 0$ for the rest); δ is the Kronecker symbol. Expression (1) are supplemented with local constraint

$$X_i^{00} + X_i^{\uparrow\uparrow} + X_i^{\downarrow\downarrow} + X_i^{22} = 1\,. \tag{2}$$

The Hamiltonian under consideration is chosen in the form

$$\begin{aligned} H = &- t_0 \sum_{\langle ij\rangle}\sum_{\sigma=\uparrow,\downarrow} X_i^{\sigma 0}X_j^{0\sigma} \\ &- t_1 \sum_{\langle ij\rangle}(X_i^{2\downarrow}X_j^{0\uparrow} + X_i^{\uparrow 0}X_j^{\downarrow 2} - X_i^{2\uparrow}X_j^{0\downarrow} - X_i^{\downarrow 0}X_j^{\uparrow 2}) \\ &- t_2 \sum_{\langle ij\rangle}\sum_{\sigma=\uparrow,\downarrow} X_i^{2\sigma}X_j^{\sigma 2} - t_3 \sum_{\langle ij\rangle} X_i^{20}X_j^{02} + U\sum_i X_i^{22} \\ &- \mu \sum_i (X_i^{\uparrow\uparrow} + X_i^{\downarrow\downarrow} + 2X_i^{22}), \end{aligned} \tag{3}$$

where t_0, t_1, t_2, and t_3 are the hopping overlap integrals: U is the interaction energy of two electrons occupying the same site; μ is a chemical potential; $\langle ij\rangle$ denotes a nearest-neighbor pair of lattice sites. The system consists of N_e electrons on the chain with N_a sites (N_a is assumed to be even). It is clear that this form of interaction conserves the individual number M and $N_e - M$ of electrons with spin up and spin down.

According to (3) if $t_0 = t_1 = t_2$ and $t_3 = 0$ the model coincides with the well-studied Hubbard model [3,8,9]. Unfortunately, such a complex model is not integrable in general for arbitrary parameters of interactions and we consider the special cases of integrability of the model only.

First of all we calculate the two-electron scattering matrix which satisfies the Yang-Baxter equations. Let us now consider the solution of the problem for the chain which contains two electrons. The general state can be written as

$$\begin{aligned} |\Psi\rangle_{\sigma_1\sigma_2} = \sum_{n_1,n_2=1}^{N_a} &[\psi_{\sigma_1\sigma_2}(n_1,n_2)X_{n_1}^{\sigma_1 0}X_{n_2}^{\sigma_2 0} \\ &+ \delta_{n_1n_2}\varphi(n_1)(\delta_{\sigma_1\uparrow}\delta_{\sigma_2\downarrow} - \delta_{\sigma_1\downarrow}\delta_{\sigma_2\uparrow})X_{n_1}^{20}]|0\rangle, \end{aligned} \tag{4}$$

where σ_1 and σ_2 are the spins of the electrons.

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The $\psi_{\sigma_1\sigma_2}(n_1,n_2)$ and $\varphi(n_1)$ amplitudes in (4) satisfy the Schrödinger equation $H|\Psi\rangle_{\sigma_1\sigma_2} = E|\Psi\rangle_{\sigma_1\sigma_2}$ which can be rewritten in the following form:

$$-t_1(\delta_{\sigma_1\uparrow}\delta_{\sigma_2\downarrow} - (\delta_{\sigma_1\downarrow}\delta_{\sigma_2\uparrow})[\psi_{\sigma_1\sigma_2}(n+1,n) + \psi_{\sigma_1\sigma_2}(n-1,n) + \psi_{\sigma_1\sigma_2}(n,n+1) + \psi_{\sigma_1\sigma_2}(n,n-1)] + U\varphi(n) - t_3[\varphi(n+1) + \varphi(n-1)] = E\varphi(n), \quad (5)$$

for $n_1 = n_2 \pm 1$,

$$-t_0[\psi_{\sigma_1\sigma_2}(n \pm 2,n) + \psi_{\sigma_1\sigma_2}(n \pm 1, n \mp 1)] - t_1(\delta_{\sigma_1\uparrow}\delta_{\sigma_2\downarrow} - \delta_{\sigma_1\downarrow}\delta_{\sigma_2\uparrow})[\varphi(n) + \varphi(n \pm 1)] = E\psi_{\sigma_1\sigma_2}(n \pm 1,n), \quad (6)$$

for $n_1 \neq n_2 \pm 1$ and $n_1 \neq n_2$,

$$-t_0[\psi_{\sigma_1\sigma_2}(n_1+1,n_2) + \psi_{\sigma_1\sigma_2}(n_1-1,n_2) + \psi_{\sigma_1\sigma_2}(n_1,n_2+1) + \psi_{\sigma_1\sigma_2}(n_1,n_2-1)] = E\psi_{\sigma_1\sigma_2}(n_1,n_2). \quad (7)$$

According to Eqs. (5) and (6) the electrons forming a triplet state are not scattered while they are scattered if their spins form a singlet state. The solution for the amplitude $\psi_{\sigma_1\sigma_2}(n_1,n_2)$ can be sought as linear combinations of two waves with wave numbers k_1 and k_2:

$$\psi_{\sigma_1\sigma_2}(x_1,x_2) = \sum_P A_{\sigma_1\sigma_2}(Q,P)\exp[i(k_{P1}x_{Q1} + k_{P2}x_{Q2})], \quad (8)$$

where $Q = (Q1,Q2)$ and $P = (P1,P2)$ are the two permutations of the integers 1 and 2; x_1 and x_2 are the coordinates of the particles. The energy which corresponds to this state equals to

$$E = -2t_0(\cos k_1 + \cos k_2) - 2\mu. \quad (9)$$

According to (7) if the interelectron distance exceeds lattice constant the electrons do not interact and the components of the tensor $A\sigma_1\sigma_2(Q,P)$ may be arbitrary. From Eq. (6) the solution for the $\varphi(n)$ amplitude in terms of the $\psi_{\sigma_1\sigma_2}(n,n)$ amplitude (its singlet part) can be written as follows:

$$\varphi(n) = t_0/(2t_1)[\psi_{\uparrow\downarrow}(n,n) - \psi_{\downarrow\uparrow}(n,n)]. \quad (10)$$

Substituting this solution into (5) and taking into account the notation of the $\psi_{\sigma_1\sigma_2}(n_1,n_2)$ amplitude in form (8) we obtain the solution for the two-particle scattering matrix, denoted as the S matrix. Unfortunately, the S matrix satisfies the Yang-Baxter equation for special values of the interaction strengths only. We write the two-particle scattering matrix for these special cases

$$S_{12} = \frac{\vartheta(k_1) - \vartheta(k_2) \pm iP_{12}}{\vartheta(k_1) - \vartheta(k_2) \pm i}, \quad (11)$$

where $t_1^2 = t_0^2/2$; $t_2t_0 = t_1^2$; for case (a) $\vartheta(k) = \frac{1}{2}\tan(k/2)$ if $t_3 = -t_0/2$, $U = t_0$ and for case (b) $\vartheta(k) = \frac{1}{2}\cot(k/2)$ if $t_3 = t_0/2$, $U = -t_0$; P_{ij} is the spin permutation operator. Later we shall use the upper and lower signs for cases (a) and (b), respectively.

The S matrix is similar to that of the t-J model but differs in the signs in Eq. (11). It means the S matrix (11) is determined by a repulsive interaction between particles.

The periodic boundary conditions imposed on the Bethe function can be expressed in terms of the T_j matrix of the model considered

$$T = S_{jj+1}S_{jj+2}\cdots S_{jN_e}S_{j1}S_{j2}S_{jj-1}. \quad (12)$$

The diagonalization of the T_j matrix is achieved by purely algebraic procedure based on the algebra of the monodromy matrix. The eigenvalues of the T_j matrix coincide with those of the Hamiltonian (3).

The Bethe ansatz equations are written in terms of the rapidities $\vartheta_j = \vartheta(k_j)$ and λ_α

$$\left(\frac{\vartheta_j - i/2}{\vartheta_j + i/2}\right)^{N_a} = \prod_{\alpha=1}^{M}\frac{\vartheta_j - \lambda_\alpha + i/2}{\vartheta_j - \lambda_\alpha - i/2}, \quad (13)$$

$$\prod_{j=1}^{N_e}\frac{\lambda_\alpha - \vartheta_j + i/2}{\lambda_\alpha - \vartheta_j - i/2} = -\prod_{\beta=1}^{M}\frac{\lambda_\alpha - \lambda_\beta + i}{\lambda_\alpha - \lambda_\beta - i}. \quad (14)$$

The energy and the magnetization of the system in the state corresponding to the sets of solutions $\{\vartheta_j\}$ and $\{\lambda_\alpha\}$ are

$$E = \pm 2N_e \mp \sum_{j=1}^{N_e}\frac{1}{\vartheta_j^2 + 1/4} - HM_z - \mu N_e, \quad (15)$$

$$M_z = \frac{N_e}{2} - M, \quad (16)$$

where H is an external magnetic field.

We shall here briefly summarize the results of the exact solution in one dimension; the details are deferred to a separate publication [10].

The structure of the solutions of the Bethe ansatz equations is similar to the one for the model of fermion gas with a repulsive delta-function interaction [11]. Asymptotical solutions of Eqs. (13) and (14) within the limit $N_a \to \infty$, are in complex plane and form strings

$$\lambda_\alpha^{nj} = \lambda_\alpha^n + i(n+1-2j)/2 + O(\exp(-\delta N_a)); \quad j = 1,2,\ldots,n; \quad \delta > 0, \quad (17)$$

which are characterized by a common real abscissa λ_α^n and the string length n. In the thermodynamic limit (with N_e/N_a, M/N_a fixed and $N_a \to \infty$) the sets of solutions $\{\vartheta_j\}$ and $\{\lambda_\alpha\}$ have real solutions for the ground state of the model. Complex spin rapidities (17) correspond

to excited states. We define distribution functions $\rho(\vartheta)$ and $\sigma_n(\lambda)$ for particles and the hole functions $\rho_h(\vartheta)$ and $\sigma_{hn}(\lambda)$ for rapidities ϑ_j and λ_α^n. The lowest-energy state is obtained by filling all states with $|\vartheta| < Q$ and $|\lambda^n| < B_n$ in case (a) and $Q < |\vartheta| < \infty$ and $|\lambda^n| < B_n$ in case (b); i.e., it corresponds to filled Dirac seas [the Dirac seas consist of all momenta and strings for which $\rho(\vartheta) \neq 0$ and $\sigma_n(\lambda) \neq 0$]. The cut-off parameters (B_n and Q) are determined by the total density of electrons and magnetization per lattice site

$$n_e = N_e/N_a = \int_{-\infty}^{\infty} d\vartheta \rho(\vartheta), \tag{18}$$

$$m_e = M/N_a = \frac{n_e}{2} - \sum_{n=1}^{\infty} n \int_{-\infty}^{\infty} d\lambda \sigma_n(\lambda). \tag{19}$$

We introduce thermodynamic energies $K(\vartheta)$ and $\varepsilon_n(\lambda)$ defined as $K(\vartheta) = T \ln[\rho_h(\vartheta)/\rho(\vartheta)]$ and $\varepsilon_n(\lambda) = T \ln[\sigma_{hn}(\lambda)/\sigma_n(\lambda)]$ which satisfy the following integral equations:

$$K(\vartheta) = \pm 2 - \mu \mp 2\pi a_1(\vartheta) + Ts * \ln[n(\varepsilon_1(\vartheta))] + TR * \ln[n(-K(\vartheta))], \tag{20}$$

$$\varepsilon_1(\lambda) = -Ts * \ln[n(\varepsilon_2(\lambda))/n(-K(\lambda))], \tag{21}$$

$$\varepsilon_n(\lambda) = -Ts * \ln[n(\varepsilon_{n+1}(\lambda))n(\varepsilon_{n-1}(\lambda))], \quad \text{for} \quad n > 1, \tag{22}$$

where

$$s(\lambda) = \frac{1}{2\cosh(\pi\lambda)}, \quad R(\lambda) = a_1 * s(\lambda), \tag{23}$$

$$a_n(\lambda) = \frac{n}{2\pi} \frac{1}{\lambda^2 + (n/2)^2}, \tag{24}$$

T is the temperature; and, finally, the symbol $a * f(\lambda)$ denotes the convolution

$$a * f(\lambda) = \int_{-\infty}^{\infty} d\mu a(\lambda - \mu) f(\mu) \tag{25}$$

At equilibrium the free energy density of the system can be expressed in terms of the quasienergies:

$$F = \epsilon_0 + T \int_{-\infty}^{\infty} d\vartheta \rho_0(\vartheta) \ln[n(K(\vartheta))] + T \int_{-\infty}^{\infty} d\lambda \sigma_0(\lambda) \ln[n(\varepsilon_1(\lambda))], \tag{26}$$

where $n(\varepsilon) = [1 + \exp(\varepsilon/T)]^{-1}$ is the Fermi distribution function; ϵ_0 is the density of the ground state energy and $\rho_0(\vartheta)$ and $\sigma_0(\lambda)$ are the distribution functions for the fully filled band at $H = 0$

$$\epsilon_0 = \pm 1 - 2\mu, \tag{27}$$

$$\rho_0(\vartheta) = a_1(\vartheta) + a_3(\vartheta), \tag{28}$$

$$\sigma_0(\lambda) = a_2(\lambda). \tag{29}$$

According to Eq. (15) at $0 < n_e < 1$ in case (a) the ground state of the model becomes ferromagnetic with density of the magnetization $m_e = n_e/2$ and the density of the ground state energy

$$\epsilon_0 = \frac{2}{\pi} \frac{Q}{Q^2 + 1/4} - m_e H, \tag{30}$$

where $Q = \frac{1}{2}\tan^{-1}(\pi n_e/2)$. If $H = 0$ and $n_e = 1$ the energy density of the system is zero. This result takes place in the t-J model [4]. For case (b) in the limit $T \to 0$ the excitation energies satisfy the following equations:

$$K(\vartheta) = -2 - \mu + 2\pi a_1(\vartheta) - H/2 + \int_{-B_1}^{B_1} d\lambda a_1(\vartheta - \lambda)\varepsilon_1(\lambda), \tag{31}$$

$$\varepsilon_1(\lambda) + \int_{-B_1}^{B_1} d\lambda' a_2(\lambda - \lambda')\varepsilon_1(\lambda') = H + a_1 * K(\lambda) - \int_{-Q}^{Q} d\vartheta a_1(\lambda - \vartheta)K(\vartheta). \tag{32}$$

Note that in contrast to the t-J model the nonmagnetic ground state of the system is characterized by real solutions of charge rapidities. The ground state configuration corresponds to the filling of all states with $K(\vartheta) < 0$ and $\varepsilon_1(\lambda) < 0$. In the absence of an external magnetic field the magnetization vanishes and $B_1 = \infty$ so we obtain the following integral equation for the charge distribution function $\rho(\vartheta)$ which is analogous to (20)

$$\rho_h(\vartheta) + \rho(\vartheta) - R * \rho(\vartheta) = a_1(\vartheta). \tag{33}$$

This integral equation has analytical solution only in the cases when the band is almost full or almost empty. If the band is almost empty then Q is very large and Eq. (33) may be solved by using the standard Wiener-Hopf technique. The kernel of the integral equation (33) is factorized into the form

$$1 + \exp(-|\omega|) = G_+(\omega)G_-(\omega), \tag{34}$$

where

$$G_-(\omega) = G_+(-\omega) = \sqrt{2\pi} \left(\frac{i\omega}{2\pi e}\right)^{i\omega/2\pi} \frac{1}{\Gamma\left(\frac{1}{2} + \frac{i\omega}{2\pi}\right)}, \tag{35}$$

$G_-(\omega)$ and $G_+(-\omega)$ are functions that are analytical in the upper and lower Fourier-space half-planes; $\Gamma(x)$ is the gamma function.

After some manipulations we obtain the expression for the density of electrons as function of Q for the almost empty band

$$n_e = 2\frac{\sqrt{2}}{\pi}\int_0^\infty \frac{d\omega}{\omega}\sin(\omega/2)G_+(i\omega)\exp(-\omega Q) + \frac{\sqrt{2}}{\pi}\int_0^\infty \frac{d\omega}{\omega}\tan(\omega/2)G_+(i\omega)\exp(-2\omega Q)f(i\omega), \tag{36}$$

where

$$f(\omega) = \frac{1}{\pi}G_+(\omega) \times \int_0^\infty \frac{d\omega\prime}{\omega' - i\omega}\sin(\omega'/2)\exp(-\omega' Q)G_+(i\omega'). \tag{37}$$

For large value Q the first term in (36) dominates since the leading contribution of the last term is of the order of $(1/\pi Q)^2$. Equation (33) can be solved numerically for arbitrary filling n_e. The results are plotted in Fig. 1.

For sufficiently large magnetic field $H \geq H_c$ the ground state of the system becomes ferromagnetic. It is evident that according to (31) and (32) the point H_c corresponds to condition $B_1 = 0$; i.e., all spins are parallel. From Eqs. (31) and (32) for $0 < n_e < 1$

$$H_c = \frac{2}{Q^2 + 1/4}\left(\frac{Q}{\pi} + n_e(-Q^2 + 1/4)\right), \tag{38}$$

where $Q = \frac{1}{2}\tan^{-1}[\pi(1 - n_e)/2]$.

In summary, we have constructed a narrow-band model which generalizes the well-known Hubbard model. The integrability of the model imposes restrictions on the dimensionality and the interaction strengths. We have obtained the Bethe ansatz equations and calculated the ground state of the system for the integrable cases. This model extends the class of integrable lattice models of strongly correlated electrons.

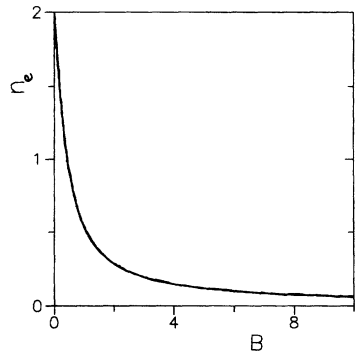

FIG. 1. The density of electrons as a function of the interaction limit B.

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