TWO CHANNELS OF SCATTERING OF HUBBARD CHAIN ELECTRONS WITH SPIN AND ORBITAL INTERACTIONS (EXACT RESULTS)

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A simple way to determine the channel of scattering of the Hubbard chain electrons with additional quantum number, which means the orbital or band characteristic, is demonstrated on the integrable 1D modified Hubbard model. Exact solutions are obtained for each scattering channel of the electrons. The preferable channel is determined by means of numerical calculations of the ground-state energies and comparison its values. The dependence of the scattering matrices on the parameters of Coulomb, orbital (band), and spin interactions gives the possibility to present the properties of the system considered in different ranges (reasonable in physics sense) of parameters which correspond to the electron coupling. The ratio between magnetic susceptibility and heat capacity of the model is presented.

PACS: 71.10.Fd; 71.10.Pm

1. INTRODUCTION

Michel Gaudin admitted that the expression "exactly soluble model" means no more than suitable mathematical expression for some physical value or at least a possibility to reduce the problem to the problem, which can be considered in a frame of classical analyses. These solutions illustrate common principles and permit to control the approximations of realistic and sophisticated models. Therefore a way to sophistication of initially exactly solved model [1] aims both the mathematical beauty and physical reality.

The interest to the exactly solvable Hubbard's chain of the electrons is high especially. It is stipulated for modern achievements both as the fundamental investigations of the nature of the super conductivity, and as the direct applications of these investigations. For example strong correlations in solids are effectively described by the Hubbard's model. The real objects for this model in condensed matter are narrow-zone transition metals. Hubbard's model describes effectively the correlations between spin and Coulomb interactions in these solids.

It is well known that at the weak Coulomb interaction limit Hubbard's model describes the non-localized spin state and Fermi-liquid behavior of the electron system. At the limit of strong Coulomb interaction Hubbard's model describes the state of localized magnetic moments of an electrons. Hence the situation which arisen in the case of intermediate ratio between the parameters of Coulomb interaction and a hopping integral is most interesting from a physical point of view. In this case it is possible to describe the phenomena of metal-dielectric phase transition, arising of local magnetic moments, correlation between the charge carriers and magnetic ordering, etc. Exact solutions of the based on the Hubbard's model problems are promising in these aspects.

The classical exact solution of the Hubbard's chain of electrons [1] does not describe the effective attraction of the electrons. Therefore it is impossible to construct the mechanism of the super conductivity in the frame of the model [1]. Some modifications of the Hubbard's model are presented in a number of works. The modifications, which are most interesting for physical interpretations permit to change effective constant of Coulomb interaction.

The effective attraction between the electrons arises in the many-band Hubbard's model, which was considered the two-band Fermi-gas model with square dispersion and δ-like potential. It takes into account the orbital and spin interactions between bands and neglects the Coulomb one.

The most interesting field of the applications of the integrable models results is high-temperature superconductivity investigations.

The models [2, 3] permit to describe more physical properties than the initial exactly solved model [1]. In the work [3] exact solution of fermionic gas two-bands model describing a parabolic band of conducting electrons and a band of local pairs interacting via δ-function was presented.

Listed above modifications of the Hubbard model got hopeful results on the way of description of effective attraction in the electron systems. Therefore it is interesting to investigate other many channel modifications of Hubbard chain of electrons.

The effective attraction between the electrons arises in the many-band Hubbard's model as it was admitted in the work [2], which the two-band Fermi-gas with square dispersion and delta-like potential was considered. It takes into account the orbital and spin interactions between bands and neglects the Coulomb one. The exact solutions were presented in the form of the tensor multiplication of the spin and orbital two-particles scattering matrixes. This model permits to describe more physical properties than the model [1]. The Hubbard's chain of the electrons with the Coulomb, and orbital, and spin interactions is considered in the work presented.

Below the Hubbard's chain of the electrons with Coulomb, orbital, and spin interactions is considered. The exact solutions are obtained by means of the coordinate Bethe-anzatz method on anti-symmetrical wave functions.

2. THE MODEL AND SOLUTION

PROBLEMS OF ATOMIC SCIENCE AND TECHNOLOGY. 2001, № 6, p. 380-382.

Modified on the case of additional type of the interaction (orbital or band) Hubbard chain Hamiltonian we shall consider in the form:

$$H = -\sum_{n=-N_a/2}^{N_a/2}\sum_{\sigma,\sigma'}\sum_{m,m'}[c^{+}_{nm\sigma}c_{n+1m\sigma} + c^{+}_{n+1m\sigma}c_{nm\sigma} -$$

$$- bc^{+}_{nm\sigma}c^{+}_{nm'\sigma'}c_{nm'\sigma'}c_{nm\sigma} - 4Uc^{+}_{nm\sigma}c_{nm\sigma}c^{+}_{nm'\sigma'}c_{nm'\sigma'}]. \quad (1)$$

Here N_a+1 denotes the number of the sites; $c^{+}_{nm\sigma}$ and $c_{nm\sigma}$ denotes operators of the creation and annihilation of electrons in the *n-th* site of the *m-th* band ($m=1,2$) with *z*-component of the spin σ ($\sigma=\uparrow,\downarrow$); value of the hopping integral we put equal to 1. The problem of the integrability of the Hamiltonian (1) is complicated in comparison with the problem [1] because a degeneracy on the second quantum number. Common approach to solve this problem leads to necessity to introduce new system of quantum characteristics, which are analogous to that of charge and spin rapidities, and a construction of three-particle system of quantum equations, which would describe the excitations of the system considered. It is way to get the wave function of the system (1) by the coordinate Bethe-anzatz in this case using two-particle scattering matrices. The procedure is described near.

We have found the solution of the Schrödinger equation for two-particle wave function

$$\Psi^{m_1m_2}_{\sigma_1\sigma_2}(n_1n_2)=f^{m_1m_2}_{\sigma_1\sigma_2}(n_1n_2)c^{+}_{n_1m_1\sigma_1}c^{+}_{n_2m_2\sigma_2}\Phi,$$

where function $f^{m_1m_2}_{\sigma_1\sigma_2}(n_1n_2)$ is the amplitude of the wave function, which satisfies the equation

$$-f^{m_1m_2}_{\sigma_1\sigma_2}(n_1+1n_2)-f^{m_1m_2}_{\sigma_1\sigma_2}(n_1-1n_2)-f^{m_1m_2}_{\sigma_1\sigma_2}(n_1n_2+1)-$$

$$-f^{m_1m_2}_{\sigma_1\sigma_2}(n_1n_2-1)+2b(1+P^{m})f^{m_1m_2}_{\sigma_1\sigma_2}(n_1n_2)\Psi_{12}-$$

$$+2Uf^{m_1m_2}_{\sigma_1\sigma_2}(n_1n_2)\Psi_{12}=Ef^{m_1m_2}_{\sigma_1\sigma_2}(n_1n_2).$$

Here permutation operators $(P^{m})^2=1$, $P^{m}=-P^{\Psi}$, and E is the energy of the system (see below). The solution of this equation gives the following cases of exact solubility of the problem and the following scattering matrices, (a) the case $U=b$

$$S^{m}_{ij}(k_i,k_j)=\frac{\sin k_i-\sin k_j+2ibP^{m}_{ij}}{\sin k_i-\sin k_j+2ib},$$

$$S^{\sigma}_{ij}(k_i,k_j)=\frac{\sin k_i-\sin k_j-2ibP^{\sigma}_{ij}}{\sin k_i-\sin k_j+2ib}; \quad (2)$$

and (b) the case $U=-b$

$$S^{m}_{ij}(k_i,k_j)=\frac{\sin k_i-\sin k_j+2ibP^{m}_{ij}}{\sin k_i-\sin k_j-2ib},$$

$$S^{\sigma}_{ij}(k_i,k_j)=\frac{\sin k_i-\sin k_j-2ibP^{\sigma}_{ij}}{\sin k_i-\sin k_j-2ib}. \quad (3)$$

Here P^{a}_{ij} denotes the permutation operator of the *i-th* and *j-th* electrons with the spin σ in the case when $a=\sigma$, and is the number of the band (orbital number) *m*, when $a=m$. All four matrices satisfy the Yang-Baxter triangle equations; therefore we can declare the model is integrable. Energy of the considered system is

$E=-2(\cos k_1+\cos k_2)$.

The whole system wave function is:

$$\Psi(Q)=\sum_{P}A(Q/P)\exp\{i\sum_{j=1}^{N_e}k_{Pj}x_{Qj}\}.$$

Here x_{Qj} are the coordinates of electrons, $x_{Q1}<x_{Q2}<\ldots<x_{QN}<L$, L is the length of the chain; Q is permutation operator of the symbols $\{1,2,\ldots N_e\}$. Construction of the transfer matrix from the scattering matrices (Eqs. (2-3)), and calculation of the eigenvalues of this matrix, which coincide with the eigenvalues of the Hamiltonian (1), reduce the problem to the diagonalization of transfer matrix.

Realization of the scattering channel in our consideration means that the quantum number of the other one is fixed. In other words the variables will divide. Each one of the equations (2) and (3) describe the special channel of scattering. It is clear, that real one will be determined by the lowest value of the ground-state energy. Therefore to calculate it we have to get the Bethe equations. To calculate the ground-state energies we get the Bethe equations as:

$$e^{ik_jN_a}=\prod_{i=1}^{N_e}\frac{\sin k_i-\sin k_j-2ib}{\sin k_i-\sin k_j+2ib}\cdot$$

$$\cdot\prod_{\beta=1}^{M}\frac{\sin k_j-\lambda_\beta-ib}{\sin k_j-\lambda_\beta+ib},$$

$$\prod_{j=1}^{N_e}\frac{\sin k_j-\lambda_\alpha-ib}{\sin k_j-\lambda_\alpha+ib}=-\prod_{\beta=1}^{M}\frac{\lambda_\alpha-\lambda_\beta+2ib}{\lambda_\alpha-\lambda_\beta-2ib}. \quad (4)$$

Here Ψ denotes a rapidities; N_e denotes the number of the electrons; M denotes the number of electrons in the spin state "down" [2, 3].

We get the system of equations, which describes the densities of a distribution of wave numbers $\Psi(k)$, and spin rapidities $\Psi(\Psi)$ in the continuum limit. Eqs. (4) are common for all four channels of a scattering. They describe the density of the rapidity distribution and may be written as:

$$\Psi\Psi(\Psi)=b\int_{-Q}^{Q}\frac{\rho(k)dk}{b^2+(\lambda-\sin k)^2}-2b\int_{-B}^{B}\frac{\sigma(\lambda')d\lambda'}{4b^2+(\lambda-\lambda')^2}.$$

Here the limits of the integration in the case of half filled chain ($N_a=N_e$) are determined by the conditions [1] and are equal toQ□□, B□¥ in the case of ground state, as it follows from the Lieb-Mattis theorem. We shall consider this case.

For the functions of the density of the momentum distribution we get:

$$2\Psi\Psi_1^{m}=1+2b\cos k\int_{-\infty}^{\infty}\frac{\sigma_m(\lambda)d\lambda}{b^2+(\lambda-\sin k)^2},$$

$$2\Psi\Psi_1^{\Psi}=1-2b\cos k\int_{-\infty}^{\infty}\frac{\sigma_m(\lambda)d\lambda}{b^2+(\lambda-\sin k)^2}+$$

$$+4b\cos k\int_{-\pi}^{\pi}dk'\frac{\rho_\sigma(k')}{4b^2+(\sin k'-\sin k)^2},$$

$$2\Psi\Psi_2^{\Psi}=1-2b\cos k\int_{-\infty}^{\infty}\frac{\sigma_m(\lambda)d\lambda}{b^2+(\lambda-\sin k)^2},$$

$$2\Psi\Psi_2^{m}=1+2b\cos k\int_{-\infty}^{\infty}\frac{\sigma_m(\lambda)d\lambda}{b^2+(\lambda-\sin k)^2}-$$

$$-4b\cos k\int_{-\pi}^{\pi} dk' \frac{\rho_\sigma(k')}{4b^2+(\sin k'-\sin k)^2}.$$

Here we denote ρ the densities, which are the orbital ones if $\sigma=m$, $a=1$ and if $\sigma=\sigma$, $a=1$, the spin ones in the case when $U=b$, and $\sigma=m$, σ, $a=2$, in the case when $U=-b$ correspondingly.

At numerical calculation of the energies of the ground state we get the following result:

– in the case when the scattering is described by the Eqs. (2) the spin channel is preferable;

– in the case when the scattering is described by the Eqs. (3) the orbital channel is preferable.

3. THERMODYNAMIC PROPERTIES OF THE MODEL

Let us consider the thermodynamic properties of the model considered in the case when the spin channel of a scattering is realized, namely the scattering matrices of Eqs. (2). Thermodynamic potential of the system will be as:

$$\frac{\Omega}{N_a}=E_0 T\int_{-\infty}^{\infty} d\lambda\,\sigma_0(\lambda)\ln n(\varepsilon_1(\lambda))+T\int_{-\pi}^{\pi} dk\rho_0(k)\ln n(K(k)), \quad (5)$$

where $n(E) = (1+\exp\{E/T\})^{-1}$ denotes the Fermi-Dirac distribution function of the electrons with the energy E, temperature T; $\rho_0(k)$, $\sigma_0(\sigma)$ are the distribution functions on the rapidities σ and momentum k consequently when $N_a=N_e$ and $T=0$:

$$\rho_0(k) = (2\pi)^{-1}(1+\cos k\int_{-\pi}^{\pi} dk' R(\sin k-\sin k')(1+2\pi\rho(k))),$$

$$\sigma_0(\sigma)=(2\pi)^{-1}\int_{-\pi}^{\pi} dk s(\sigma-\sin k)(1+2\pi\rho(k))$$

Here $s(\sigma) = (4b\cosh\pi\sigma/b)^{-1}$, and $R(x)$ is the Fourier transformed function $R(\sigma) = (1+\exp\{2\pi\sigma/b\})^{-1}$. Functions $K(k)$ and $\varepsilon_i(\lambda)$ satisfies the set of the integral equations which appears in the classical Hubbard problem [4] (i=1,2):

$$K(k) = -2\cos k+H-4\int_{-\infty}^{\infty} d\sigma s(\sin k-\sigma)\sigma\sqrt{1-(\lambda+ib)^2}$$

$$+T\int_{-\infty}^{\infty} d\sigma s(\sin k-\sigma)\sigma\ln\frac{n(\varepsilon_1(\lambda))}{n(\varepsilon_1'(\lambda))},$$

$$\varepsilon_i(\lambda)=-Ts\ln(n(\varepsilon_{i+1}(\lambda))n(\varepsilon_{i-1}(\lambda)))+$$

$$+T\pi_{i1}\int_{-\pi}^{\pi} dk\cos k s(\sin k-\sigma)\ln n(-K(k))$$

Here H denotes the amplitude of external magnetic field. Boundary conditions for this case we choose as:

$$\lim_{i\to\infty}\frac{\varepsilon_i(\lambda)}{i}=2H;\ \varepsilon_0(\lambda)=-\infty.$$

Here symbol $\cdot$ denotes the convolution:

$$sf=\int ds(\sigma-p)f(p).$$

In the limit of weak external magnetic field $H\to 0$ the magnetic susceptibility we get as:

$$\chi^{Hub}=\frac{SUI_0(a)}{\pi^2 I_1(a)}[1+(N\ln|H|)^{-1}-\frac{\ln|\ln|H||}{(N\ln|H|)^2}+\ldots].$$

Here $I_0(a)=\int dk e^{a\sin k}\rho(k)$, $I_1(a)=-(1/2)\int dk\cos k e^{a\sin k}\rho(k)$, $a=4\pi/NU$ and functions $\rho(k)$, $\sigma(k)$ calculate from the well-known procedure [1]. The result is

$$\chi^{Hub}=\frac{UI_0(a)}{4I_1(a)}\chi^{HC},$$

where χ^{HC} is the heat capacity of the Heisenberg chain was presented in the work [5]. This capacity satisfy the following conditions in the case N=2:

$$\lim_{T\to 0}\lim_{H\to 0}\chi^{HC}=2/3,$$

$$\lim_{H\to 0}\lim_{T\to 0}\chi^{HC}=(1/3)(1+(\sqrt{2})^{1/2}).$$

In our case minimal value of the number N=4 (when we have two orbits or bands). Therefore we have to consider 4 integral Bethe anzatz equations. But due to our approximation we may consider each channel of a scattering separately and use the above results.

Hence we can write

$$\frac{\gamma^{Hub}}{\gamma}=\frac{\chi^{Hub}}{\chi}=I_0(\frac{\pi}{2b}).$$

4. CONCLUSIONS

Presented way of the separation of the channels of a scattering of Hubbard chain electrons model permits to reduce effective constant of Coulomb interaction in Hubbard's model due to the consideration of orbital scattering channel of the electrons.

The modification of the Hubbard model on the case of existing in the system of the strong correlated electrons two channels of a scattering gives the exact values of the modification parameter b, which makes the model Hamiltonian integrable. It is interesting to admit that the region of integrability is defined by the equality of the values of a modification parameter and model Coulomb interaction.

Hence, the mechanisms of the realization of the transitions from different magnetic states, metal-insulator transition, etc., in 1D integrable strong correlated electron quantum systems, which are described by the Hamiltonian Eq. (1) will be determinate by the parameters of 4-fermionic interaction.

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