Quantum phase transition and elementary excitations of a Bose-Fermi mixture in a one-dimensional optical lattice

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The mixture of the scalar bosonic and the spinless or polarized fermionic cold atoms in the one-dimensional optical lattice is studied. The system is modeled by the Bose-Fermi-Hubbard Hamiltonian, which shows different behavior from that of the Bose-Hubbard or the Fermi-Hubbard models. Because the SU(1|1)-supersymmetric Bethe ansatz solution gives an excellent approximation to this kind of mixed cold atomic systems, the ground-state properties of the system such as the densities of state in the momentum space are obtained based on the Bethe ansatz. If the number of bosons is equal to that of fermions and the filling factor is 1, it is found that there exists a critical on-site interaction U_c. If $U < U_c$, the ground state of the system is in the superfluid phase, while if $U > U_c$, the ground state is in the insulating phase. The superfluid-insulator transition occurs at U_c. From the analysis of the superfluid density, the value of the critical point is determined as $U_c = 2.79256$, which is larger than the $U_c = 0$ for the Fermi-Hubbard model and smaller than the $U_c = 3.28$ for the Bose-Hubbard model. The elementary excitations and effective Hamiltonian in the strong-coupling limit are also discussed.

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I. INTRODUCTION

Recently, the cold atoms in the optical lattices catch the attentions for many novel states of matter are found in this kind of systems.[1,2] By using the magnetic fields or laser beams, the cold atoms can be trapped in the one-dimensional (1D) optical lattice.[3–10] With Feshbach resonance, the scattering length and the interactions among the atoms can be manipulated. The rapid development of the experimental techniques for cold atoms provide us a platform to study some controllable condensed-matter systems. The Bose-Fermi mixtures of cold atoms in the optical lattice is a remarkable research topic. Experimenters have succeeded in preparing the Bose-Fermi mixtures such as ^{7}Li-^{6}Li,[11,12] ^{23}Na-^{6}Li,[13,14] ^{87}Rb-^{40}K,[15–20] ^{87}Rb-^{6}Li,[21] and ^{3}He-^{4}He.[22] Many interesting phenomena such as the phase separations driven by hopping and the quantum phase transition driven by interactions are observed in the mixture.[23,24]

The low-energy physics of cold atomic gas can be described by the continue models quite well.[25–34] Some continue models such as Lieb-Liniger model,[35,36] two-component bosons model,[37] spin-1/2 fermions model,[38] the atoms gas with exchanging interactions,[39,40] and the mixture of the spin-1/2 fermions and the scalar bosons model[41,42] are exactly solvable. The exact solution can supply some believable results thus serves as a very good starting point to understand the new phenomena and new quantum states in trapped cold atomic systems.

The two-component fermionic cold atoms in the 1D optical lattice are described by the Fermi-Hubbard model, which can be solved exactly.[43] The exact solution shows that the system is a insulator at zero temperature for any nonzero interactions. The bosonic cold atoms in the 1D optical lattice are described by the Bose-Hubbard model.[44] Unlike the Fermi-Hubbard model, the Boson-Hubbard model can not be solved exactly, even at the cases that there are no more than two atoms occupying the same site.[45–47] Thus many numerical methods dealing with the many-body systems such as density-matrix renormalization group,[48] quantum Monte Carlo simulations,[49,50] and exact diagonalization[51] are applied to the Bose-Hubbard model. The approximation based on the mean-field theory such as Bogoliubov-de Gennes theory and Gross-Pitaevskii equation are also used. The hard-core Bose-Hubbard model has the exact solution[52,53] since the behavior of the hard-core bosons is like that of the fermions although the symmetries are different. The hard-core bosons and fermions can be mapped into each other by the Jordan-Wigner transformation or the Bose-Fermi mapping.

In the Bose-Hubbard model, if the on-site interaction U is very small, the ground state of the system is a superfluid state for the atoms can hop in the optical lattice easily. While if the on-site interaction U is very large, the strong repulsive interactions prohibit the hopping of atoms, thus the system is in the insulating phase. The superfluid-insulator phase transition happens at the critical point U_c. The value of U_c is determined as $U_c = 3.28 \pm 0.04$ by the quantum Monte Carlo simulation[54] and $U_c = 2\sqrt{3}$ by the Bethe ansatz approximation.[55] This property is very different from that of the Fermi-Hubbard model, where the critical values is $U_c = 0$.[43] Then it is natural to ask what will happen if we replace all the spin-down fermions by the scalar bosons, where the new system can be modeled by the Bose-Fermi-Hubbard model. What is the new quantum state in the mixture system? These issues are interesting and important nowadays due to the rapid progress in the field of cold atomic physics.

In this paper, we study a mixture of scalar bosons and spinless or polarized fermions in the 1D optical lattice. In Refs. 56–58, it is shown that the Bose-Fermi Hubbard model has the supersymmetry invariance. We find that if the hopping of the atoms are equal and the interactions among the bosons and that among the fermion and bosons are equal, the

SU(1|1)-invariant Bethe ansatz solution is a very good approximation solution of the system. This argument can be understood easily at two obvious cases: dilute cold atoms gas and strong repulsive interaction, for the multi-occupied situations in these two cases are very rare. Therefore, we construct the SU(1|1)-supersymmetric solution with different gradings by using the coordinate Bethe ansatz and the graded quantum inverse scattering method.[59–63] We consider the case of $U>0$ that is the interaction is repulsive. By solving the Bethe ansatz equations, we obtain the densities of state in the momentum at the ground state. We find that the ground state of present Bose-Fermi-Hubbard model has a phase transition at the nonzero critical point U_c. The system is in the superfluid phase if $U<U_c$ while is in the insulating phase if $U>U_c$. The value of U_c is determined as $U_c=2.79256\pm 0.00448$, which is larger than $U_c=0$ for the Fermi-Hubbard model and smaller than $U_c=3.28$ for the Bose-Hubbard model.

The paper is organized as follows. In Sec. II, we derive the two-body SU(1|1)-invariant scattering matrix by using the coordinate Bethe ansatz method. In Sec. III, we derive the Bethe ansatz solution by using the graded quantum inverse scattering method. Base on this excellent approximation solution, we discuss the ground-state properties and the quantum phase transition in Sec. IV. In Sec. V, we discuss the low-lying excitations of the system. The effective Hamiltonian in the strong-coupling limit and other gradings cases are shown in the Secs. VI and VII, respectively. Section VIII contains some conclusions and discussions.

II. SYSTEM

The mixture of the scale bosons and the spinless or polarized fermions in the 1D optical lattice can be described by the Bose-Fermi-Hubbard model with the Hamiltonian

$$H=-\sum_{j=1}^{L}(t_b b_j^\dagger b_{j+1}+\text{H.c.})-\sum_{j=1}^{L}(t_f f_j^\dagger f_{j+1}+\text{H.c.})+\frac{U_{bb}}{2}\sum_{j=1}^{L}n_{b,j}(n_{b,j}-1)+U_{bf}\sum_{j=1}^{L}n_{b,j}n_{f,j}, \tag{1}$$

where t_b is the hopping of bosons, t_f is the hopping of fermions, $b_j^\dagger(b_j)$ is the bosonic creating (annihilating) operator at the site j, $f_j^\dagger(f_j)$ is the fermionic creating (annihilating) operators at the site j, U_{bb} is the interaction among the bosons, U_{bf} is the interaction between the bosons and fermions, and L is the number of total sites. Due to the Pauli exclusive principle, two fermions can not occupy the same positions, thus Hamiltonian (1) does not include the interaction among the fermions. Denote the number of bosons as N_b, the number of fermions as N_f, and the total number of atoms as $N=N_b+N_f$. In this paper, we consider the system with the periodic boundary conditions and the interactions are repulsive.

In Ref. 64, Albus, Illuminati, and Eisert introduce the Bose-Fermi-Hubbard model and derive the explicit Hamiltonian from the microscopic many-body Hamiltonian, linking the experimentally accessible quantities to the model parameters. They also give the conditions for linear stability of the model and derive a mean-field criterion for the onset of a bosonic superfluid transition in the ground state, using the Gutzwiller formulation and numerical analysis of finite systems.[64] The ground-state phase diagram of the Bose-Fermi-Hubbard model is obtained by using the exact numerical solution[65,66] and the analytical methods.[67] The superfluid and Mott-insulator transition is studied with the quantum Monte Carlo simulations using the canonical worm algorithm.[68] The pairing in the system with equal densities and unequal masses is studied in the framework of numerical density-matrix renormalization group.[69] The phase diagram of homogeneous boson-fermion mixtures in optical lattices is studied in Ref. 70, and the ground-state properties of inhomogeneous mixtures in cubic lattices and parabolic confining potentials are studied in Ref. 71. In the inhomogeneous system and for finite hopping, the domain boundaries between Mott-insulator plateaux and hopping-dominated regions for lattices of arbitrary dimension are also determined within mean-field and perturbation theory.[71] In Ref. 72, Illuminati and Albus predict the high-temperature superfluidity of the fermionic atoms induced by the boson-fermion interaction.

The system, Eq. (1), is not integrable for the Bethe ansatz scattering matrix can not exactly describe the scattering process of more than two particles occupying the same site. However, the SU(1|1)-supersymmetric Bethe ansatz solution is a very good approximation solution of the system.[55,73] This argument can be understood as following. In the dilute cold atoms gas, the situation of multi-atom occupying the same site is quite rare. Meanwhile, if the repulsive interaction is very strong, the system also favors the state that every site are occupied by one particles. In these cases, the Bethe ansatz solution are very close to the actual values as expected. In fact, the Bethe ansatz solutions in other cases are also quite good comparing the mean-field theory.[55,73] This might because that even at the multi-occupying case, the Bethe ansatz scattering matrix catch the dominate scattering process and neglect the high-order scattering processes which can be regarded as corrections. For the single and double occupations, the Bethe ansatz is exact and the corrections are zero. Meanwhile, the probability of the bosons occupy the same site in the experimental setup is very small, thus the Bethe ansatz solution can describe the physics of the bosonic atoms in the optical lattice.

In order to construct the SU(1|1)-supersymmetric Bethe ansatz solution, we should consider the case that the hopping of bosons and fermions are equal, $t_b=t_f=t$, which is set to unity in the following. Meanwhile the interactions among the bosons U_{bb} and the interaction between boson and fermion U_{bf} are also equal, $U_{bb}=U_{bf}=U$. The wave functions of the system is symmetry if we exchanging two bosons while is antisymmetry if we exchanging two fermions.

In the framework of coordinate Bethe ansatz, we assume the many-particles eigenstates of the system, Eq. (1), as

$$|\Psi\rangle=\sum_{x_1\dots x_N}\Psi(x_1,\dots,x_N)b_{x_1}^\dagger\dots b_{x_{N_b}}^\dagger f_{x_{N_b+1}}^\dagger\dots f_{x_N}^\dagger|0\rangle, \tag{2}$$

where $|0\rangle$ means the vacuum state of the system and $\Psi(x_1,\dots,x_N)$ is the wave function. Not losing generality, we suppose that first N_b coordinates belong to the bosons and the wave functions at this part is symmetric, while the next N_f coordinates belong to the fermions and the wave function at this part is asymmetric. Solving the static Schrödinger equation $H|\Psi\rangle=E|\Psi\rangle$, we obtain following eigenequation

$$-\sum_{j=1}^{N}[\Psi(x_1,\ldots,x_j+1,\ldots x_N)+\Psi(x_1,\ldots x_j-1,\ldots,x_N)] + U\sum_{j<l}\delta_{x_jx_l}\Psi(x_1,\ldots,x_N)=E\Psi(x_1,\ldots,x_N). \quad (3)$$

Using Bethe's hypothesis, we suppose that the wave function of the system, Eq. (1), is described by a set of quasimomenta $\{k_j\}$ as[35,38,39,43]

$$\Psi(x_1\ldots x_N)=\sum_{Q,P}\theta(x_{Q_1}<\cdots<x_{Q_N})A(Q,P)e^{i\sum_{j=1}^{N}k_{P_j}x_{Q_j}}, \quad (4)$$

where $Q=(Q_1,\ldots,Q_N)$ and $P=(P_1,\ldots,P_N)$ are the permutations of the integers $1,\ldots,N$, N is the total number of particles, $\theta(x_{Q_1}<\cdots<x_{Q_N})=\theta(x_{Q_N}-x_{Q_{N-1}})\ldots\theta(x_{Q_2}-x_{Q_1})$ and $\theta(x-y)$ is the step function, and $A(Q,P)$ is the amplitude of the wave function.

If the coordinates of quasiparticles in the assumed state, Eq. (2), are not equal, $x_1\neq x_2\neq\cdots\neq x_N$, the eigenequation (3) can be solved analytically by the Fourier transformation. After some algebra, we obtain the energy spectrum as

$$E=-2\sum_{j=1}^{N}\cos k_j, \quad (5)$$

where k_j are the quasimomentum which are determined by the periodic boundary conditions. The effective two-body scattering exist in the case that two quasiparticle occupy the same site. To explore the two-body scattering mechanics, we consider two regimes

$$Q_1{:}0<x_{Q_1}<x_{Q_2}<x_{Q_3}<x_{Q_4}<\cdots<x_{Q_N}<L,$$

$$Q_2{:}0<x_{Q_1}<x_{Q_3}<x_{Q_2}<x_{Q_4}<\cdots<x_{Q_N}<L.$$

Suppose the wave functions in the regimes Q_1 and Q_2 are Ψ_1 and Ψ_2, respectively. If $x_{Q_2}=x_{Q_3}=x$ and all other coordinates are not equal, that is to say only the site x is double occupied, from the static Schrödinger equation, we obtain

$$\begin{aligned}&-[\Psi_2(\ldots x+1\ldots x\ldots)+\Psi_1(\ldots x-1\ldots x\ldots)\\&\quad+\Psi_1(\ldots x\ldots x+1\ldots)+\Psi_2(\ldots x\ldots x-1\ldots)]\\&\quad-\sum_{j\neq Q_2,Q_3}[\Psi_1(\ldots x_j+1\ldots)+\Psi_1(\ldots x_j-1\ldots)]\\&\quad+U\Psi_1(\ldots x\ldots x\ldots)=Ef_1(\ldots x\ldots x\ldots).\end{aligned} \quad (6)$$

The wave function are continuous, $\Psi_1(\ldots x\ldots x\ldots)=\Psi_2(\ldots x\ldots x\ldots)$. Substituting the ansatz of wave function, Eq. (4), into the continuous conditions of wave function, we have

$$A(Q^{(1)},P^{(2)})-A(Q^{(2)},P^{(1)})=A(Q^{(2)},P^{(2)})-A(Q^{(1)},P^{(1)}), \quad (7)$$

where $P^{(1)}=(P_1P_2P_3P_4\ldots P_N)$ and $P^{(2)}=(P_1P_3P_2P_4\ldots P_N)$. On the other hand, if all the coordinates in the regime Q_1 are not equal, we have

$$-\sum_{j}[\Psi_1(\ldots x_j+1\ldots)+\Psi_1(\ldots x_j-1\ldots)]=E\Psi_1(x_1\ldots x_N). \quad (8)$$

Equation (8) can be rewritten as

$$\begin{aligned}&-[\Psi_1(\ldots x+1\ldots x\ldots)+\Psi_1(\ldots x\ldots x-1\ldots)\\&\quad+\Psi_1(\ldots x\ldots x+1\ldots)+\Psi_1(\ldots x-1\ldots x\ldots)\\&\quad-\sum_{j\neq Q_2,Q_3}[\psi_1(\ldots x_j+1\ldots)+\Psi_1(\ldots x_j-1\ldots)]\\&=E\Psi_1(x_1\ldots x\ldots x\ldots x_N),\end{aligned} \quad (9)$$

where $\Psi_1(\ldots x+1\ldots x\ldots)$ and $\Psi_1(\ldots x\ldots x-1\ldots)$ are values of wave function in the regime Q_2, which are denoted as $\Psi_1^c(\ldots x+1\ldots x\ldots)$ and $\Psi_1^c(\ldots x\ldots x-1\ldots)$. From Eqs. (6) and (9), we have

$$\Psi_1^{(c)}(\ldots x+1\ldots x\ldots)-\Psi_2(\ldots x+1\ldots x\ldots)+\Psi_1^{(c)}(\ldots x\ldots x-1\ldots)-\Psi_2(\ldots x\ldots x-1\ldots)+U\Psi_1(\ldots x\ldots x\ldots)=0. \quad (10)$$

Substituting the ansatz of wave function, Eq. (4), into Eq. (10), we obtain

$$\begin{aligned}&[A(Q^{(1)},P^{(1)})-A(Q^{(2)},P^{(2)})](e^{ik_{P_2}}+e^{-ik_{P_3}})\\&\quad+[A(Q^{(1)},P^{(2)})-A(Q^{(2)},P^{(1)})](e^{ik_{P_3}}+e^{-ik_{P_2}})\\&\quad+U[A(Q^{(1)},P^{(1)})+A(Q^{(2)},P^{(2)})]=0.\end{aligned} \quad (11)$$

The compact form of Eq. (11) is

$$A(Q,\ldots P_2P_3\ldots)=Y^{23}_{P_3P_2}A(Q,\ldots P_3P_2\ldots), \quad (12)$$

$$Y^{23}_{P_3P_2}=\frac{(\sin k_{P_2}-\sin k_{P_3})P_{Q_2Q_3}+i\frac{U}{2}}{\sin k_{P_2}-\sin k_{P_3}-i\frac{U}{2}}. \quad (13)$$

Using the similar technique, we obtain the general relations of scattering process of arbitrary two sites, $A(Q,\ldots lj\ldots)=Y^{ab}_{jl}A(Q,\ldots jl\ldots)$, where $Y^{ab}_{jl}=[(\sin k_l-\sin k_j)P_{Q_aQ_b}+iU/2]/[\sin k_l-\sin k_j-iU/2]$. The two-body scattering matrix is $S_{jl}(k_j-k_l)=P_{Q_aQ_b}Y^{ab}_{jl}$, which can be written out explicitly

$$S_{jl}(k_j-k_l)=\frac{\sin k_j-\sin k_l-i\frac{U}{2}P^s_{jl}}{\sin k_j-\sin k_l+i\frac{U}{2}}, \quad (14)$$

where P^s_{jl} is the super permutation operator with the definition $[P^s_{jl}]^{\beta\nu}_{\alpha\mu}=(-1)^{\epsilon_\alpha\epsilon_\beta}\delta_{\alpha\nu}\delta_{\mu\beta}$, the α and μ are the row indices, and β and ν are the column indices. Here ϵ_α is the Grassmann number, $\epsilon_a=0$ for bosons and $\epsilon_a=1$ for fermions. The scattering matrix satisfies the super or graded Yang-Baxter equation[59–62]

$$S_{12}(k_1-k_2)S_{13}(k_1-k_3)S_{23}(k_2-k_3) = S_{23}(k_2-k_3)S_{13}(k_1-k_3)S_{12}(k_1-k_2). \quad (15)$$

The indices form of the Yang-Baxter equation (15) is

$$S_{12}(k_1-k_2)^{b_1b_2}_{a_1a_2}S_{13}(k_1-k_3)^{c_1b_3}_{b_1a_3}S_{23}(k_2-k_3)^{c_2c_3}_{b_2b_3} \times(-1)^{(\epsilon_{b_1}+\epsilon_{c_1})\epsilon_{b_2}} = S_{23}(k_2-k_3)^{b_2b_3}_{a_2a_3} \times S_{13}(k_1-k_3)^{b_1c_3}_{a_1b_3}S_{12}(k_1-k_2)^{c_1c_2}_{b_1b_2}(-1)^{(\epsilon_{a_1}+\epsilon_{b_1})\epsilon_{b_2}}.$$

With the periodic boundary conditions, we obtain following eigenvalue equations

$$S_{jN}(k_j-k_N)S_{jN-1}(k_j-k_{N-1})\ldots S_{jj+1}(k_j-k_{j+1}) \times S_{jj-1}(k_j-k_{j-1})\ldots S_{j1}(k_j-k_1)e^{ik_jL}\xi_0=\xi_0, \quad (16)$$

where ξ_0 is the amplitude of initial-state wave function.

III. BETHE ANSATZ SOLUTIONS

The eigenvalue, Eq. (16), can be solved exactly by using the graded quantum inverse scattering method. There are two ways to choose the Grassmann parities. One is $\epsilon_1=0$ and $\epsilon_2=1$, which corresponds the bosonic-fermionic (BF) grading. The other is $\epsilon_1=1$ and $\epsilon_2=0$, which corresponds the fermionic-bosonic (FB) grading. In the graded algebra Bethe ansatz method, choosing different gradings is equivalent to choosing different highest weight represents in the deriving of Bethe ansatz solutions. The form of Bethe ansatz equations for different gradings may be different. The Bethe ansatz equations with different gradings can change into each others by using some gauge transformations.[61]

A. BF grading

We first consider the BF grading. The Lax operator of jth site in the auxiliary space reads

$$S_j(\lambda)=\begin{pmatrix} a(\lambda)-b(\lambda)e^{11}_j & -b(\lambda)e^{21}_j \\ -b(\lambda)e^{12}_j & a(\lambda)+b(\lambda)e^{22}_j \end{pmatrix}, \quad (17)$$

where the matrix $e^{\alpha\beta}_j$ acts on the jth quantum space with the elements $(e^{\alpha\beta}_j)_{\mu\nu}=\delta_{\alpha\mu}\delta_{\beta\nu}$, $a(\lambda)=\lambda/[\lambda+iU/2]$, and $b(\lambda)=iU/2[\lambda+iU/2]$. For simplicity, we introduced the R matrix $R_{12}(\lambda)=P^s_{12}S_{12}(\lambda)$, which satisfies the braid Yang-Baxter equation

$$R_{12}(\lambda-u)R_{23}(\lambda)R_{12}(u)=R_{23}(u)R_{12}(\lambda)R_{23}(\lambda-u). \quad (18)$$

The monodromy matrix of the system is constructed by the Lax operators as

$$T_N(\lambda)=S_j(\lambda-\sin k_j)S_N(\lambda-\sin k_N)\ldots S_{j+1}(\lambda-\sin k_{j+1})S_{j-1}(\lambda-\sin k_{j-1})\ldots S_1(\lambda-\sin k_1) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda)\end{pmatrix}, \quad (19)$$

where $A(\lambda)$, $B(\lambda)$, $C(\lambda)$, and $D(\lambda)$ are the operators defined in the N quantum spaces. From Eq. (18), we can prove that the monodromy matrix satisfies the Yang-Baxter relation

$$R_{12}(\lambda-u)[T_N(\lambda)\otimes_s T_N(u)]=[T_N(u)\otimes_s T_N(\lambda)]R_{12}(\lambda-u), \quad (20)$$

where $\otimes_s$ means the super or graded tensor product as $[A\otimes_s B]^{bd}_{ac}=(-1)^{(\epsilon_a+\epsilon_b)\epsilon_c}A_{ab}B_{cd}$, a and c are the row indices, and b and d are the column indices. Using indices method, the Yang-Baxter relation (20) can also be written as

$$R_{12}(\lambda-u)^{b_1b_2}_{a_1a_2}T_N(\lambda)^{c_1}_{b_1}T_N(u)^{c_2}_{b_2}(-1)^{(\epsilon_{b_1}+\epsilon_{c_1})\epsilon_{b_2}} = T_N(u)^{b_1}_{a_1}T_N(\lambda)^{b_2}_{a_2}R_{12}(\lambda-u)^{c_1c_2}_{b_1b_2}(-1)^{(\epsilon_{a_1}+\epsilon_{b_1})\epsilon_{a_2}}, \quad (21)$$

where all the repeated indices should be summed. The elements of scattering matrix $S_{ij}(\lambda)^{b_1b_2}_{a_1a_2}$ are nonzero only at three conditions: (1) $a_1=a_2=b_1=b_2$, (2) $a_1=b_1$, $a_2=b_2$, and (3) $a_1=b_2$, $a_2=b_1$. These properties will be used in deriving the commutation relations. The transfer matrix $t(\lambda)$ of the system is defined as the supertrace of the monodromy matrix in the auxiliary space

$$t(\lambda)=str_0T_N(\lambda)=A(\lambda)-D(\lambda), \quad (22)$$

where 0 means the auxiliary space. From the Yang-Baxter relation (20), we can prove that the transfer matrices with different spectral parameters commute with each other, $[t(u),t(v)]=0$. The eigenvalue problem, Eq. (16), is therefore reduced to

$$-str_0T_N(k_j)e^{ik_jL}\xi_0=\xi_0, \quad (23)$$

We choose the local vacuum state as $|0\rangle_j=(0,1)^t$, where t means the transpose. The Lax operator acting on this vacuum state gives

$$S_j(\lambda)|0\rangle_j=\begin{pmatrix} a(\lambda-\sin k_j) & 0 \\ * & 1\end{pmatrix}|0\rangle_j, \quad (24)$$

where * represents a nonzero value. The global vacuum state is constructed as $|0\rangle=\otimes^N_{j=1}|0\rangle_j$. Acting the monodromy matrix, Eq. (19), on this vacuum state, we have

$$T_N(\lambda)|0\rangle=\begin{pmatrix} \prod_{j=1}^N a(\lambda-\sin k_j) & 0 \\ C(\lambda) & 1\end{pmatrix}|0\rangle. \quad (25)$$

The elements $A(\lambda)$ and $D(\lambda)$ acting on the vacuum state give the eigenvalues. The element $B(\lambda)$ acting on the vacuum state is zero. The element $C(\lambda)$ acting on the vacuum state gives nonzero value and can be regarded as the creation operator. We assume the eigenstates of the system, Eq. (1), are obtained by applying the creation operator $C(\lambda)$ on the vacuum state as

$$|\Psi\rangle=C(\lambda_1)C(\lambda_2)\ldots C(\lambda_M)|0\rangle, \quad (26)$$

where M is the number of creating operators. When the transfer matrix acting on the Bethe states, Eq. (26), we need the commutation relations between $A(\lambda)$, $D(\lambda)$, and $C(\lambda)$. From the Yang-Baxter relation (21) and using the properties of R matrix, we find following commutation relations

$$A(\lambda)C(u)=\frac{a(\lambda-u)-b(\lambda-u)}{a(\lambda-u)}C(u)A(\lambda)+\frac{b(\lambda-u)}{a(\lambda-u)}C(\lambda)D(u), \qquad (27)$$

$$D(\lambda)C(u)=\frac{1}{a(u-\lambda)}C(u)D(\lambda)-\frac{b(u-\lambda)}{a(u-\lambda)}C(\lambda)D(u), \qquad (28)$$

$$C(\lambda)C(u)=[a(\lambda-u)-b(\lambda-u)]C(u)C(\lambda). \qquad (29)$$

The elements $C(\lambda)$ and $C(u)$ do not commute with each other, which is very different form that of the Fermi-Hubbard model.

The transfer matrix acting on the assumed states gives two kinds of terms. One is the eigenvalue and others are the unwanted terms. If the assumed states are the eigenstates of the transfer matrix, the unwanted terms must be cancelled with each other, which determines the values of parameters in the ansatz (26). Acting the transfer matrix, Eq. (22), on the assumed Bethe states, Eq. (26), applying repeatedly the commutation relations (27)–(29) and using the result (25), we obtain

$$t(u)C(\lambda_1)\ldots C(\lambda_M)|0\rangle=\left\{\prod_{l=1}^{M}\frac{a(u-\lambda_l)-b(u-\lambda_l)}{a(u-\lambda_l)}\times\prod_{j=1}^{N}a(u-\sin k_j)-\prod_{l=1}^{M}\frac{1}{a(\lambda_l-u)}\right\}\times C(\lambda_1)\ldots C(\lambda_M)|0\rangle+u.t., \qquad (30)$$

where $u.t.$ means the unwanted terms. If the unwanted terms are cancelled with each other, that is to say if the following Bethe ansatz equations are satisfied

$$\prod_{\alpha=1,\neq\beta}^{M}\frac{1}{a(\lambda_\alpha-\lambda_\beta)}\frac{a(\lambda_\beta-\lambda_\alpha)}{a(\lambda_\beta-\lambda_\alpha)-b(\lambda_\beta-\lambda_\alpha)}=\prod_{l=1}^{N}a(\lambda_\beta-\sin k_l),\quad \beta=1,2,\ldots,M, \qquad (31)$$

the assumed state, Eq. (26), is the eigenstate of the transfer matrix and the first term in Eq. (30) is the eigenvalue of the transfer matrix $t(u)$. From the eigenvalues Eq. (16) we obtain the second set of the Bethe ansatz equations as

$$e^{ik_jL}=\prod_{\alpha=1}^{M}a(\lambda_\alpha-\sin k_j),\quad j=1,\ldots,N. \qquad (32)$$

Putting $\lambda_\alpha\to\lambda_\alpha-iU/4$, then Eqs. (31) and (32) take the form of

$$e^{ik_jL}=\prod_{\alpha=1}^{M}\frac{\sin k_j-\lambda_\alpha+i\frac{U}{4}}{\sin k_j-\lambda_\alpha-i\frac{U}{4}},\quad j=1,\ldots,N, \qquad (33)$$

$$\prod_{l=1}^{N}\frac{\lambda_\beta-\sin k_l-i\frac{U}{4}}{\lambda_\beta-\sin k_l+i\frac{U}{4}}=1,\quad \beta=1,\ldots,M, \qquad (34)$$

where $N=N_b+N_f$ and $M=N_b$. The Bethe ansatz equations (33) and (34) are different from that of the Fermi-Hubbard model, and also different from that of the SU(2) Bose-Hubbard model. To our knowledge, the Bethe ansatz equations (33) and (34) are never proposed before.

Taking the logarithm of Eqs. (33) and (34), we arrive at

$$k_jL=2\pi I_j-2\sum_{\alpha=1}^{N_b}\theta_{1/4}(\sin k_j-\lambda_\alpha),$$

$$\pi J_\beta=\sum_{l=1}^{N}\theta_{1/4}(\lambda_\beta-\sin k_l), \qquad (35)$$

where $\theta_\gamma(x)=\tan^{-1}[x/(\gamma U)]$ and the quantum numbers I_j and J_β take integer or half-odd integer values, depending on whether N and N_b are even or odd, respectively. The energy E and the momentum P are

$$E=-2\sum_{j=1}^{N}\cos k_j,\quad P=\sum_{j=1}^{N}k_j. \qquad (36)$$

B. FB grading

Now we consider the FB grading. The Lax operator of jth site is

$$S_j(\lambda)=\begin{pmatrix}a(\lambda)+b(\lambda)e_j^{11} & -b(\lambda)e_j^{21}\\ -b(\lambda)e_j^{12} & a(\lambda)-b(\lambda)e_j^{22}\end{pmatrix}. \qquad (37)$$

The monodromy matrix of the system is constructed by the Lax operator as

$$T_N(\lambda)=S_j(\lambda-\sin k_j)S_N(\lambda-\sin k_N)\ldots S_{j+1}(\lambda-\sin k_{j+1})S_{j-1}(\lambda-\sin k_{j-1})\ldots S_1(\lambda-\sin k_1)=\begin{pmatrix}A(\lambda) & B(\lambda)\\ C(\lambda) & D(\lambda)\end{pmatrix}, \qquad (38)$$

which satisfies the Yang-Baxter relation

$$R_{12}(\lambda-u)[T_N(\lambda)\otimes_s T_N(u)]=[T_N(u)\otimes_s T_N(\lambda)]R_{12}(\lambda-u), \qquad (39)$$

where $R_{12}(\lambda)=P_{12}^sS_{12}(\lambda)$. The transfer matrix $t(\lambda)$ of the system is defined as the supertrace of the monodromy matrix, Eq. (38),

$$t(\lambda)=strT_N(\lambda)=-A(\lambda)+D(\lambda). \qquad (40)$$

We choose the local vacuum state as $|0\rangle_j=(0,1)^t$. The global vacuum state is $|0\rangle=\otimes_{j=1}^{N}|0\rangle_j$. Acting the monodromy matrix on the global vacuum state, we have

$$A(\lambda)|0\rangle=\prod_{l=1}^{N}a(\lambda-k_l)|0\rangle, \qquad (41)$$

$$B(\lambda)|0\rangle = 0, \quad C(\lambda)|0\rangle \neq 0, \tag{42}$$

$$D(\lambda)|0\rangle = \prod_{l=1}^{N} [a(\lambda - \sin k_l) - b(\lambda - \sin k_l)]|0\rangle. \tag{43}$$

The elements $A(\lambda)$ and $D(\lambda)$ acting on the vacuum state give the eigenvalues. The element $B(\lambda)$ acting on the vacuum state is zero. The element $C(\lambda)$ acting on the vacuum state gives nonzero value and can be regarded as the creating operator. We assume the eigenstates of the system, Eq. (1), are obtained by applying the creation operator $C(\lambda)$ on the vacuum state as

$$|\Psi\rangle = C(\lambda_1) \dots C(\lambda_M)|0\rangle, \tag{44}$$

where M is the number of creating operators. When the transfer matrix, Eq. (40), acting on the Bethe states, Eq. (44), we need the commutation relations between $A(\lambda)$, $D(\lambda)$, and $C(\lambda)$. From the Yang-Baxter relation (39), we obtain following commutation relations

$$A(\lambda)C(u) = \frac{1}{a(\lambda - u)}C(u)A(\lambda) - \frac{b(\lambda - u)}{a(\lambda - u)}C(\lambda)D(u), \tag{45}$$

$$D(\lambda)C(u) = \frac{a(u-\lambda) - b(u-\lambda)}{a(u-\lambda)}C(u)D(\lambda) + \frac{b(u-\lambda)}{a(u-\lambda)}C(\lambda)D(u), \tag{46}$$

$$C(\lambda)C(u) = \frac{-1}{a(\lambda - u) - b(\lambda - u)}C(u)C(\lambda). \tag{47}$$

Acting the transfer matrix, Eq. (40), on the assumed eigenstate, Eq. (44), applying repeatedly the commutation relations (45)–(47) and using the result (43), we have

$$t(u)|\Psi\rangle = \Lambda_{t(u)}|\Psi\rangle + u.t., \tag{48}$$

where $\Lambda_{t(u)}$ is the eigenvalues of the transfer matrix

$$\Lambda_{t(u)} = -\prod_{\alpha=1}^{M} \frac{1}{a(u-\lambda_\alpha)} \prod_{j=1}^{N} a(u - \sin k_j) + \prod_{\alpha=1}^{M} \frac{a(\lambda_\alpha - u) - b(\lambda_\alpha - u)}{a(\lambda_\alpha - u)} \times \prod_{j=1}^{N} [a(u - \sin k_j) - b(u - \sin k_j)]. \tag{49}$$

From the condition that the unwanted terms must be canceled with each other, we obtain following Bethe ansatz equations

$$e^{ik_jL} = \prod_{l=1,\neq j}^{N} \frac{\sin k_l - \sin k_j - i\frac{U}{2}}{\sin k_l - \sin k_j + i\frac{U}{2}} \times \prod_{\alpha=1}^{M} \frac{\sin k_j - \lambda_\alpha - i\frac{U}{4}}{\sin k_j - \lambda_\alpha + i\frac{U}{4}}, \quad j = 1, \dots, N, \tag{50}$$

$$\prod_{l=1}^{N} \frac{\lambda_\beta - \sin k_l + i\frac{U}{4}}{\lambda_\beta - \sin k_l - i\frac{U}{4}} = 1, \quad \beta = 1, \dots, M, \tag{51}$$

where $N=N_b+N_f$ and $M=N_f$. Taking the logarithm of Eqs. (50) and (51), we arrive at

$$k_jL = 2\pi I_j - 2\sum_{l=1}^{N} \theta_{1/2}(\sin k_j - \sin k_l) + 2\sum_{\alpha=1}^{M} \theta_{1/4}(\sin k_j - \lambda_\alpha), \tag{52}$$

$$\pi J_\beta = \sum_{l=1}^{N} \theta_{1/4}(\lambda_\beta - \sin k_l). \tag{53}$$

where the quantum numbers satisfy

$$|I_j| \leq \frac{1}{2}(N - M - 1), \quad |J_\beta| \leq \frac{1}{2}N. \tag{54}$$

Thus I_j is integer (half-odd integer) if $N-M$ is odd (even) and J_β is integer (half-odd integer) if N is even (odd). The energy E and the momentum P are

$$E = -2\sum_{j=1}^{N} \cos k_j, \quad P = \sum_{j=1}^{N} k_j. \tag{55}$$

In the thermodynamic limit, the densities of state should satisfy

$$\rho(k) = \frac{1}{2\pi} + \frac{\cos k}{\pi} \int_{-Q}^{Q} \frac{2U\rho(k')dk'}{U^2 + 4(\sin k - \sin k')^2} - \frac{1}{\pi} \int_{-B}^{B} \frac{4U\sigma(\lambda)d\lambda}{U^2 + 16(\sin k - \lambda)^2}, \tag{56}$$

$$\sigma(\lambda) = \frac{1}{\pi} \int_{-Q}^{Q} \frac{4U\rho(k)dk}{U^2 + 16(\lambda - \sin k)^2}. \tag{57}$$

The integral limits Q and B are determined by

$$\frac{N}{L} = \int_{-Q}^{Q} \rho(k)dk, \quad \frac{N_f}{L} = \int_{-B}^{B} \sigma(\lambda)d\lambda. \tag{58}$$

The energy and momentum are

$$\frac{E}{L} = -2\int_{-Q}^{Q} \cos k\rho(k)dk, \quad \frac{P}{L} = \int_{-Q}^{Q} k\rho(k)dk. \tag{59}$$

IV. GROUND STATE AND QUANTUM PHASE TRANSITION

A. Ground state

Now, we study the ground state of the system. If we use the grand canonical ensemble, the ground state of the system is composed of the bosons. Here, we consider the canonical ensemble thus the numbers of bosons and fermions are fixed. We use the BF grading as a demonstration. In this paper, we suppose $U>0$ that is to say the interaction among the atoms is repulsive. We also assume that the number of bosons is equal to that of fermions. In this case, the rapidities k and λ in the Bethe ansatz equations at the ground state are real. Taking the logarithm of Eqs. (33) and (34), we have

$$k_j L = 2\pi I_j - 2\sum_{\alpha=1}^{N_b} \tan^{-1}\left(\frac{\sin k_j - \lambda_\alpha}{U/4}\right), \qquad (60)$$

$$\pi J_\beta = \sum_{l=1}^{N} \tan^{-1}\left(\frac{\lambda_\beta - \sin k_l}{U/4}\right). \qquad (61)$$

Here the quantum number I_j is integer (half-odd integer) if N_b is even (odd) and J_β is integer (half-odd integer) N is even (odd). The total momentum is

$$K = \frac{2\pi}{L}\left[\sum_j I_j + \sum_\alpha J_\alpha\right]. \qquad (62)$$

At the ground state, I_j and J_α are successive number centered around the origin. For example,

$$I_j = -\frac{N-1}{2}, -\frac{N-3}{2}, \ldots, \frac{N-1}{2}, \qquad (63)$$

$$J_\beta = -\frac{N_b-1}{2}, -\frac{N_b-3}{2}, \ldots, \frac{N_b-1}{2}. \qquad (64)$$

We solve the Bethe ansatz equations (60) and (61) numerically. The density of state in momentum space at the ground state is shown in Fig. 1.

In the thermodynamic limit, that is all the L, N, and N_b tend to infinity but the ratios N/L and N_b/L keep finite, the summation is replaced by the integration. Define $f(k_j)=I_j/L$ and $g(\lambda_\beta)=J_\beta/L$, and we have

$$k = 2\pi f(k) - 2\int_{-B}^{B} 2\tan^{-1}\left(\frac{\sin k - \lambda}{U/4}\right)\sigma(\lambda)d\lambda, \qquad (65)$$

$$\int_{-Q}^{Q} 2\tan^{-1}\left(\frac{\lambda - \sin k}{U/4}\right)\rho(k)dk = 2\pi g(\lambda), \qquad (66)$$

where $\pm Q$ are the upper and lower bound of the distribution of ks and $\pm B$ are the bounds on the λs. Define the distribution functions of ks and λs as $\rho(k)=df(k)/dk$ and $\sigma(\lambda)=dg(\lambda)/d\lambda$, respectively. Differentiating Eq. (65) with respect to k and Eq. (66) with respect to λ, we have

$$\rho(k) = \frac{1}{2\pi} + \cos k\int_{-B}^{B} 2a_1(\sin k - \lambda)\sigma(\lambda)d\lambda, \qquad (67)$$

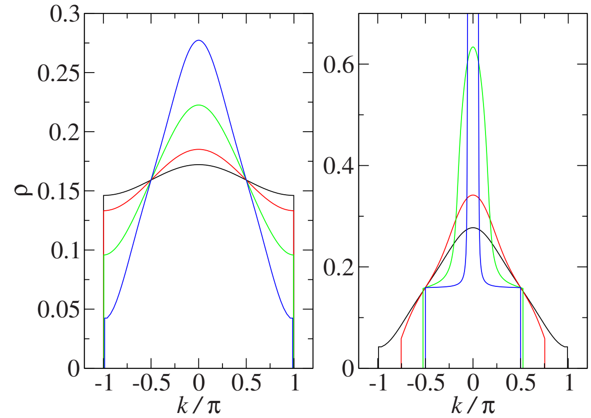

FIG. 1. (Color online) Density of state in momentum space at the ground state. Here, $N_b=N_f=99$, $U=10,5,2,1$ (left) and $U=1.0,0.5,0.1,0.01$ (right) for the lines from bottom to top at the position of $k=0$.

$$\sigma(\lambda) = \int_{-Q}^{Q} a_1(\lambda - \sin k)\rho(k)dk, \qquad (68)$$

where $a_n(x)=4nU/[\pi(n^2U^2+16x^2)]$. The values of Q and B are determined by

$$\frac{N}{L} = \int_{-Q}^{Q}\rho(k)dk, \quad \frac{N_b}{L} = \int_{-B}^{B}\sigma(\lambda)d\lambda. \qquad (69)$$

The energy and momentum are

$$\frac{E}{L} = -2t\int_{-Q}^{Q}\cos k\rho(k)dk, \quad \frac{P}{L} = \int_{-Q}^{Q} k\rho(k)dk. \qquad (70)$$

Now we consider the ground state of the system with the filling factor $N/L=1$. From Eq. (69), we obtain $\int_{-\pi}^{\pi}\rho(k)dk=1$, which means that the Fermi point is $Q=\pi$. From Eq. (69), we also have $\int_{-\infty}^{\infty}\sigma(\lambda)d\lambda=1$. Thus at the ground state, B should tend to infinity and the ground state of the system is constructed by the bosons. In this case, the densities of state can be solved by the Fourier transformation

$$\tilde{\sigma}(\omega) = \int_{-\infty}^{\infty}\sigma(\lambda)e^{-i\omega\lambda}d\lambda, \quad \sigma(\lambda) = \frac{1}{2\pi}\int_{-\infty}^{\infty}e^{i\omega\lambda}\tilde{\sigma}(\omega)d\omega.$$

Using the integration formula

$$\int_{-\infty}^{\infty}\frac{e^{-i\omega x}dx}{a^2+x^2} = \frac{\pi}{a}e^{-a|\omega|}, \quad (a>0),$$

$$\int_{-\infty}^{\infty}\frac{e^{-i\omega\lambda}d\lambda}{U^2+4(\lambda-\lambda')^2} = \frac{\pi}{2U}e^{-i\omega\lambda'-U/2|\omega|},$$

$$\int_{-\infty}^{\infty}\frac{e^{-i\omega\lambda}d\lambda}{U^2+16(\lambda-\sin k)^2} = \frac{\pi}{4U}e^{-i\omega\sin k-U/4|\omega|},$$

and taking the Fourier transformation of $\sigma(\lambda)$ [Eq. (68)], we have

$$\tilde{\sigma}(\omega) = e^{-U/4|\omega|}\int_{-\pi}^{\pi} e^{-i\omega \sin k}\rho(k)dk. \tag{71}$$

From Eq. (67), we have

$$\int_{-\pi}^{\pi} e^{-i\omega \sin k}\rho(k)dk = J_0(\omega), \tag{72}$$

where $J_0(\omega)$ is the Bessel functions. For later use, we introduce another Bessel function $J_1(\omega)$. The definitions of $J_0(\omega)$ and $J_1(\omega)$ are

$$J_0(\omega) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-i\omega \sin k}dk, \tag{73}$$

$$J_1(\omega) = \frac{\omega}{2\pi}\int_{-\pi}^{\pi} \cos^2 k \cos(\omega \sin k)dk. \tag{74}$$

Taking the inverse Fourier transformation of Eq. (71) and using Eq. (72), we have

$$\sigma(\lambda) = \frac{1}{\pi}\int_{-\infty}^{\infty} \cos(\omega\lambda)J_0(\omega)e^{-U/4|\omega|}d\omega. \tag{75}$$

Using the integration formula,

$$\int_{-\infty}^{\infty} \frac{\cos(\omega\lambda)d\lambda}{U^2 + 16(\lambda - \sin k)^2} = \frac{\pi}{4U}\cos(\omega \sin k)e^{-U/4|\omega|}, \tag{76}$$

we obtain the density of quasimomentum distribution as

$$\rho(k) = \frac{1}{2\pi} + \frac{\cos k}{\pi}\int_{-\infty}^{\infty} J_0(\omega)\cos(\omega \sin k)e^{-U/2|\omega|}d\omega. \tag{77}$$

Substituting Eq. (77) into Eq. (70), we obtain the density of ground-state energy as

$$\frac{E}{L} = -8\int_{0}^{\infty} \frac{J_0(\omega)J_1(\omega)}{\omega e^{U/2|\omega|}}d\omega. \tag{78}$$

B. Quantum phase transition and stiffness

At zero temperature, the transport properties of the 1D Bose-Fermi-Hubbard model are depend on the superfluid density. The superfluid density or the stiffness can be computed from the ground-state energy $E(\phi)$ as[74]

$$D_c = \frac{N}{2}\frac{\partial^2 E(\phi)}{\partial \phi^2}, \tag{79}$$

where ϕ is the external magnetic flux. The superfluid density is a very useful physics quantity. To our case, the system, Eq. (1), is a superfluid if D_c is finite, and is an insulator if D_c is zero. In order to study the ground-state phase diagram of the system, Eq. (1), we apply a magnetic flux ϕ to the system. It is well known that the magnetic flux ϕ piercing the system with the periodic boundary condition can be gauged out by imposing the twisted boundary condition on the system.[75,76]

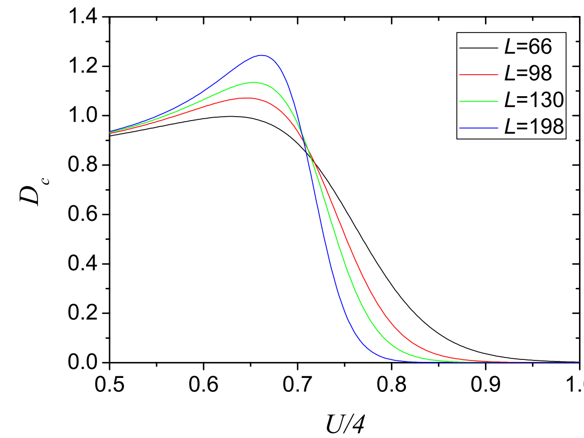

FIG. 2. (Color online) The superfluid density of the system versus the different system size.

Therefore, solving the Schrödinger equation in the presence of the magnetic flux with the periodic boundary condition is equivalent to that in the absence of the magnetic flux but with a twisted boundary condition for the wave functions $\Psi(x_1,\ldots,x_n+L,\ldots)=\Psi(x_1,\ldots,x_n,\ldots)$. Then the Bethe ansatz equations (33) and (34) become

$$k_jL = 2\pi I_j + \phi - 2\sum_{\alpha=1}^{N_b} \tan^{-1}\left(\frac{\sin k_j - \lambda_\alpha}{U/4}\right), \tag{80}$$

$$\pi J_\beta = \sum_{l=1}^{N} \tan^{-1}\left(\frac{\lambda_\beta - \sin k_l}{U/4}\right). \tag{81}$$

From the solution of Eqs. (80) and (81), we can obtain the ground-state energy of the system. Then using the Eq. (79), we obtain the superfluid density.

We restrict our studies in the case of $L=N$, which means that the filling factor is 1, and the number of bosons is equal to that of fermions, $N_b=N_f$. If the on-site interaction U is zero, all the bosons condense at the ground state in the momentum space, that is the bosons occupy the $k=0$ energy level. Due to the Pauli exclusive principle, the fermions are arranged from the lowest-energy level to the Fermi surface. If U is very small, the system is in the superfluid phase regime. Thus the jump of the superfluid density can not drop to the zero. If U is very large, the bosons become the hard-core ones. The system enters the insulating phase regime. The elementary excitations have a gap. The superfluid-insulator phase transitions happens at the critical U_c,[65] which belong to the Kosterlitz-Thouless-type phase transition. If U tends to infinity, all the atoms are frozen. The properties of the system can be well characterized by the 1D XY model with transverse magnetic fields.

The ground-state superfluid density of the 1D Bose-Fermi-Hubbard model with different system size is shown in Fig. 2. We see that the superfluid density has an inflexion. We take the derivative of superfluid density with respect to the interaction, which is shown in Fig. 3. From the Fig. 3, we see that the derivative has a minimum D'_m at a certain interaction U_m, which can be used to determine the critical point

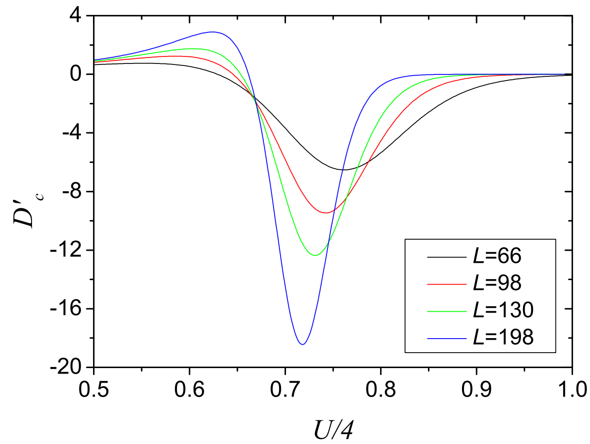

FIG. 3. (Color online) The derivative of the superfluid density of the system, which has a minimum at a certain interaction U_m.

of the system. Fig. 4 is the finite-size scaling behavior of the minimum of the derivative of the superfluid density. The data can be fitted as a straight line $D'_m=-0.60952-0.09013L$. The minimum D'_m tends to negative infinity when the system size tends to infinity. Thus D'_m is divergent at the critical point. The finite-size scaling behavior of the transition point U_m is shown in Fig. 5. From the data analysis, we obtain $U_m=2.79256+16.7696/L$. In the thermodynamic limit, U_m gives the critical point as $U_c=2.79256\pm0.00112$.

V. LOW-LYING EXCITATIONS

From the above analysis, we know that the dominant configuration at the ground state of the system is the Néel state where the bosons and fermions are arranged alternately. There exist two kinds of low-lying excitations. One is that two rapidities λ form a two string. The corresponding schematic representation of this excitations is shown in Fig. 6(I) and 6(I). In this excitation, two kinks are present in the background of the Neel state. Another excitation is that two quasimomentum k and one λ form a $k-\lambda$ string in which a doubly occupied state and one hole are present in the background of the Neel state, which is shown in Fig. 6(I), 6(I), and 6(I). In this excitation, two particles form a bound state. From the solutions of the Bethe ansatz equations, all the excitation spectrum can be calculated exactly.

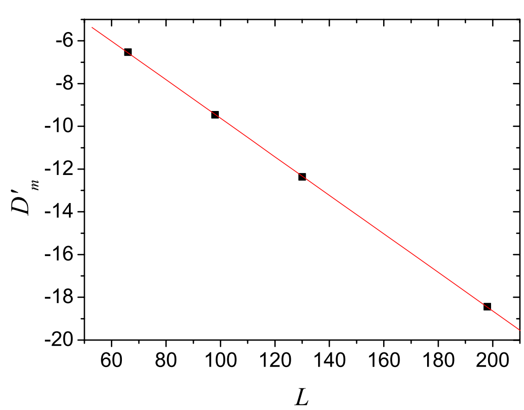

FIG. 4. (Color online) The finite-size scaling behavior of the minimum of the derivative of the superfluid density D'_m. The data can be fitted as $D'_m=-0.60952-0.09013L$. The minimum is divergence in the thermodynamic limit.

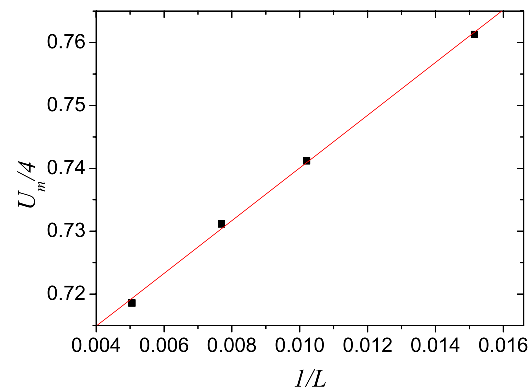

FIG. 5. (Color online) The finite-size scaling behavior of the U_m at which the derivative of the superfluid density of the system has a minimum. The data can be fitted as $U_m/4=0.69814+4.1924/L$. In the thermodynamic limit, the critical value is $U_c=2.79256\pm0.00112$.

We first consider the two-string excitation, which means that the λ sea has two holes and one two string. The λ two string can be parameterized as

$$\lambda_n=\Lambda+iU/4,\quad \lambda_m=\Lambda-iU/4, \tag{82}$$

where Λ is real. Substituting Eq. (82) into the Bethe ansatz equations (33) and (34), we obtain

$$e^{ik_jL}=\prod_{\alpha=1}^{N_b-2}\frac{\sin k_j-\lambda_\alpha+i\frac{U}{4}}{\sin k_j-\lambda_\alpha-i\frac{U}{4}}\frac{\sin k_j-\Lambda+i\frac{U}{2}}{\sin k_j-\Lambda-i\frac{U}{2}},\quad j=1,\ldots,N, \tag{83}$$

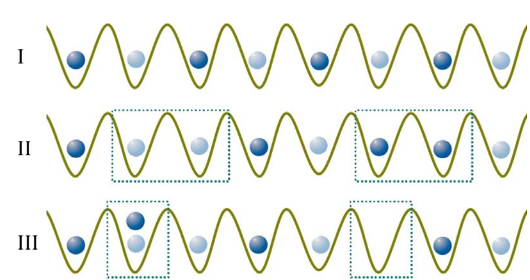

FIG. 6. (Color online) (I) The dominant configuration of the ground state in perspective of Neel state where the bosons and fermions are arranged alternately. (II) λ two-string excitation in which two kinks are present in the background of the Neel state. (III) $k-\lambda$ string excitation in which a doubly occupied state and one hole are present in the background of the Neel state. Here the dark and light particles denote fermions and bosons, respectively.

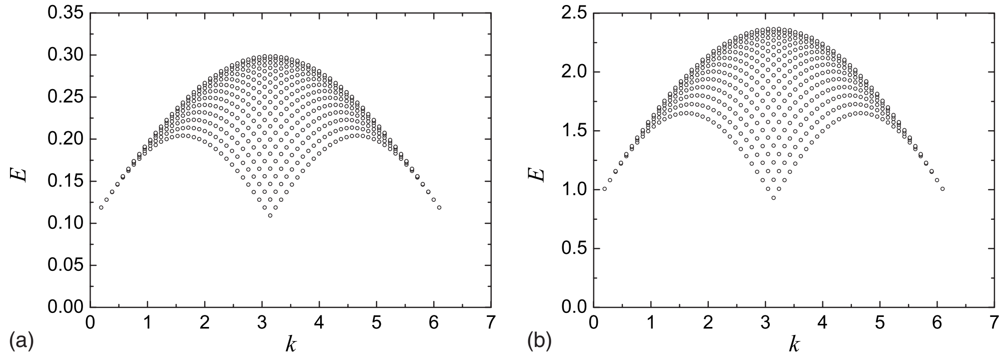

FIG. 7. The energy spectrum of the λ two-string excitation with the weak coupling $U=4$ (up) and strong coupling $U=40$ (down). Here $L=66$ and $N_b=N_f=33$.

$$\prod_{l=1}^{N}\frac{\lambda_\beta-\sin k_l-i\frac{U}{4}}{\lambda_\beta-\sin k_l+i\frac{U}{4}}=1,\quad \beta=1,\ldots,N_b-2, \tag{84}$$

$$\prod_{l=1}^{N}\frac{\Lambda-\sin k_l-i\frac{U}{2}}{\Lambda-\sin k_l+i\frac{U}{2}}=1. \tag{85}$$

Taking the logarithm of Eqs. (83)–(85), we have

$$k_jL=2\pi I_j-2\sum_{\alpha=1}^{N_b-2}\tan^{-1}\left(\frac{\sin k_j-\lambda_\alpha}{U/4}\right)-2\tan^{-1}\left(\frac{\sin k_j-\Lambda}{U/2}\right), \tag{86}$$

$$2\pi J_\alpha=2\sum_{l=1}^{N}\tan^{-1}\left(\frac{\lambda_\beta-\sin k_l}{U/4}\right), \tag{87}$$

$$2\pi K_\beta=2\sum_{l=1}^{N}\tan^{-1}\left(\frac{\Lambda-\sin k_l}{U/2}\right), \tag{88}$$

where the quantum number I_j is integer (half-odd integer) if N_b is odd (even) and the quantum numbers J_α and K_β are integers (half-odd integers) if N is even (odd). The quantum numbers are used to determine the eigenstates and the corresponding eigenvalues. At the ground state, the quantum numbers take the continue integers or half-odd integers. In the excited states, the quantum numbers no longer take the continue values. Focusing on our problem, the λ two-string excitation is characterized by the quantum number sequences

$$I_j=-\frac{N-2}{2},-\frac{N-2}{2}+1,\ldots,\frac{N}{2}, \tag{89}$$

$$J_\alpha=-\frac{N_b-1}{2},-\frac{N_b-1}{2}+1,\ldots,-\frac{N_b-1}{2}+s-1,$$

$$-\frac{N_b-1}{2}+s+1,\ldots,-\frac{N_b-1}{2}+r-1,$$

$$-\frac{N_b-1}{2}+r+1,\ldots,\frac{N_b-1}{2}-1, \tag{90}$$

$$K_\beta=0, \tag{91}$$

where $0\leq s<r\leq N_b$. The energy and momentum spectrum are given in terms of the Bethe ansatz quantum numbers as

$$E_{ex}=-\sum_{j=1}^{N}2\cos k_j, \tag{92}$$

$$P=\frac{2\pi}{L}\left(\sum_j I_j+\sum_\alpha J_\alpha+\sum_\beta K_\beta\right). \tag{93}$$

The excited energy is $E=E_{ex}-E_{gs}$, where E_{gs} is the ground-state energy. By solving the Bethe ansatz equations (86)–(88), we obtain the excited-state energy E_{ex}. Meanwhile, by solving Eqs. (33) and (34), we obtain the ground-state energy E_{gs}. Subtracting E_{gs} from E_{ex}, we obtain the excited energy E for this two-string excitation, which is shown in Fig. 7.

In the thermodynamic limit, the summations become integrations. The quantum number I_j and J_α become continue functions of the spectral parameters k and λ, respectively. Denote the density of momentum k as $\rho(k)$, the density of rapidities λ as $\sigma(\lambda)$, and the density of λ holes as $\sigma^h(\lambda)$. Then we have $\rho(k)=dI_j/(Ldk)$ and $\sigma(\lambda)+\sigma^h(\lambda)=dJ_a/(Ld\lambda)$. Taking the derivative of Eqs. (86)–(88), we conclude that these densities of states should satisfy the integral Bethe ansatz equations

$$\rho(k)=\frac{1}{2\pi}+\cos k\int a_1(\sin k-\lambda)\sigma(\lambda)d\lambda+\frac{1}{L}a_2(\sin k-\Lambda)\cos k, \tag{94}$$

$$\sigma(\lambda)+\sigma^h(\lambda)=\int a_1(\lambda-\sin k)\rho(k)dk, \tag{95}$$

$$\sigma_2(\Lambda) = \int a_2(\Lambda - \sin k)\rho(k)dk, \tag{96}$$

where $\sigma_2(\Lambda')=\delta(\Lambda'-\Lambda)/L$ is the density of the two string, $\sigma^h(\lambda)=[\delta(\lambda-\lambda_1^h)+\delta(\lambda-\lambda_2^h)]/L$, and λ_1^h and λ_2^h are the positions of the holes. From the ground-state distributions $\rho(k)$ and $\sigma(\lambda)$, we obtain the differences of the densities of states between the ground state and the excited state as

$$\Delta k\rho(k) = \int a_1(\sin k - \lambda)\Delta\lambda\sigma(\lambda)d\lambda + \frac{1}{L}a_2(\sin k - \Lambda)\Delta\Lambda,$$

$$\Delta\lambda[\sigma(\lambda) + \sigma^h(\lambda)] = \int \cos k\Delta k\rho(k)a_1(\lambda - \sin k)dk,$$

$$\Delta\Lambda\sigma_2(\Lambda) = \int \cos k a_2(\Lambda - \sin k)\Delta k\rho(k)dk.$$

Thus the excited energy E is

$$E = E_{ex} - E_{gs} = 2L\int \sin k\rho(k)\Delta k dk. \tag{97}$$

Next, we consider the two-particle bound state, that is the $k-\lambda$ excitation with the form of

$$k_n = \pi - \sin^{-1}(\Lambda + iU/4), \tag{98}$$

$$k_m = \pi - \sin^{-1}(\Lambda - iU/4), \tag{99}$$

where Λ is real. Substituting Eqs. (99) and (98) into the Bethe ansatz equations (33) and (34), we obtain

$$e^{ik_jL} = \prod_{\alpha=1}^{N_b-1} \frac{\sin k_j - \lambda_\alpha + i\frac{U}{4}}{\sin k_j - \lambda_\alpha - i\frac{U}{4}} \frac{\sin k_j - \Lambda + i\frac{U}{4}}{\sin k_j - \Lambda - i\frac{U}{4}}, \tag{100}$$

$$e^{i(k_n+k_m)L} = \prod_{\alpha=1}^{N_b-1} \frac{\Lambda - \lambda_\alpha + i\frac{U}{2}}{\Lambda - \lambda_\alpha - i\frac{U}{2}} \times \prod_{l=1}^{N-2} \frac{\Lambda - \sin k_l + i\frac{U}{4}}{\Lambda - \sin k_l - i\frac{U}{4}}, \tag{101}$$

$$\prod_{l=1}^{N-2} \frac{\lambda_\beta - \sin k_l - i\frac{U}{4}}{\lambda_\beta - \sin k_l + i\frac{U}{4}} \frac{\lambda_\beta - \Lambda - i\frac{U}{2}}{\lambda_\beta - \Lambda + i\frac{U}{2}} = 1, \tag{102}$$

where $j=1,\ldots,N-2$ and $\beta=1,\ldots,N_b-1$. The logarithm form of Eqs. (100)–(102) are

$$k_jL = 2\pi I_j - 2\sum_{\alpha=1}^{N_b-1} \tan^{-1}\left(\frac{\sin k_j - \lambda_\alpha}{U/4}\right) - 2\tan^{-1}\left(\frac{\sin k_j - \Lambda}{U/4}\right), \quad j=1,\ldots,N-2, \tag{103}$$

$$2\mathcal{I}[\sin^{-1}(\Lambda + iU/4)]L = 2\sum_{\alpha=1}^{N_b-1} \tan^{-1}\left(\frac{\Lambda - \lambda_\alpha}{U/2}\right) + 2\pi J_\alpha + 2\sum_{l=1}^{N-2} \tan^{-1}\left(\frac{\Lambda - \sin k_l}{U/4}\right), \tag{104}$$

$$2\pi K_\beta = 2\sum_{l=1}^{N-2} \tan^{-1}\left(\frac{\lambda_\beta - \sin k_l}{U/4}\right) + 2\tan^{-1}\left(\frac{\lambda_\beta - \Lambda}{U/2}\right), \quad \beta = 1,\ldots,N_b-1, \tag{105}$$

where $\mathcal{I}$ means the imaginary part, the quantum number I_j is integer (half-odd integer) if N_b is even (odd), J_α is integer (half-odd integer) if $N+N_b-5$ is even (odd), and K_β is integer (half-odd integer) if $N-1$ is even (odd). In the $k-\lambda$ excitation, the quantum number sequence I_j has two holes. Without losing generality, we suppose the positions of holes are r and s. The quantum number sequence K_β has one hole with the position t. Meanwhile, the quantum number of the string composed of two k and one λ should be treated alone. After detailed analysis, we find that the quantum numbers in this excitation should take the values of

$$I_j = -\frac{N-1}{2}, -\frac{N-1}{2}+1, \ldots, -\frac{N-1}{2}+s-1,$$

$$-\frac{N-1}{2}+s+1, \ldots, -\frac{N-1}{2}+r-1,$$

$$-\frac{N-1}{2}+r+1, \ldots, \frac{N-1}{2}-1,$$

$$J_\alpha = \frac{1}{2},$$

$$K_\beta = -\frac{N_b-1}{2}, \ldots, -\frac{N_b-1}{2}+t-1,$$

$$-\frac{N_b-1}{2}+t+1, \ldots, \frac{N_b-1}{2},$$

where $\leq s < r \leq N_b$. The excited energy E can be calculated exactly by the solution of Eqs. (103)–(105) as

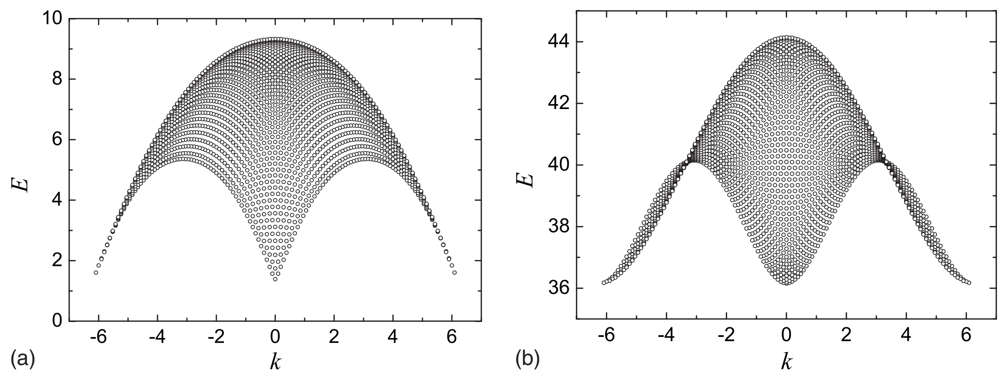

FIG. 8. The energy spectrum of the $k-\lambda$ string excitation with the weak coupling $U=4$ (up) and strong coupling $U=40$ (down). Here $L=66$ and $N_b=N_f=33$.

$$E=E_{ex}-E_{gs}=-\sum_{j=1}^{N-2} 2\cos k_j+4\mathcal{R}\sqrt{1-(\Lambda-iU/4)^2}-E_{gs},$$

where $\mathcal{R}$ refers to the real part. The results are shown in Fig. 8. We see that the excitation spectrum has a energy gap, which is consistent with the fact that the system in the strong-coupling limit is a quantum XY model with a transverse field.

In the thermodynamic limit, we introduce the densities of holes

$$\rho^h(k)=\frac{1}{L}[\delta(k-k_1^h)+\delta(k-k_2^h)], \tag{106}$$

$$\sigma^h(\lambda)=\frac{1}{L}\delta(\lambda-\lambda^h), \tag{107}$$

where k_1^h and k_2^h are the positions of holes in the distribution of quasimomentum k, and λ^h is the position of hole in the distribution of rapidity λ. Then the densities of state in this excitation should satisfy the integral Bethe ansatz equations

$$\rho(k)+\rho^h(k)=\frac{1}{2\pi}+\int a_1(\sin k-\lambda)\sigma(\lambda)d\lambda+\frac{1}{L}a_1(\sin k-\Lambda), \tag{108}$$

$$\sigma'(\Lambda)=2\mathcal{R}\left[\frac{1}{\sqrt{1+(\Lambda+iU/4)^2}}\right]-\int a_2(\Lambda-\lambda)\times\sigma(\lambda)d\lambda-\int a_1(\Lambda-\sin k)\cos k\rho(k)dk, \tag{109}$$

$$\sigma(\lambda)+\sigma^h(\lambda)=\int a_1(\lambda-\sin k)\cos k\rho(k)dk+\frac{1}{L}a_2(\lambda-\Lambda), \tag{110}$$

where $\sigma'(\Lambda')=\delta(\Lambda'-\Lambda)/L$ and $\Lambda=(\sin k_1^h+\sin k_2^h)/2$. The solution of Eqs. (108)–(110) gives the excited energy as

$$E=-2L\int\cos k\rho(k)dk+4\mathcal{R}\sqrt{1-(\Lambda-iU/4)^2}-E_{gs}.$$

VI. STRONG-COUPLING LIMIT

If the filling factor is 1 and the number of bosons is equal to that of fermions, every site will have one particle in the strong-coupling limit. The quasimomentum rapidities k_j in the charge sector are frozen and the main contribution comes from the spin rapidities λ_α in the spin sector. The system is equivalent to an anisotropic quantum spin chain in the strong-coupling limit. There are many methods such as quantum inverse scattering method,[77] Schriffer-Wolf transformation[78] and the one suggested in Ref. 79 to derive the effective Hamiltonian of the system. We first use the quantum inverse scattering method. The starting point is the scattering matrix, Eq. (17), and the transfer matrix, Eq. (22), in the spin sector. Taking the derivative of the logarithms of the transfer matrix, Eq. (22), with respect to the spin rapidity λ, we obtain the effective Hamiltonian of the system in the strong-coupling limit with the BF grading

$$H=-\frac{1}{2}\sum_{j=1}^{N}(\sigma_j^x\sigma_{j+1}^x+\sigma_j^y\sigma_{j+1}^y+2\sigma_j^z). \tag{111}$$

It is nothing but the 1D quantum ferromagnetic XY model with transverse magnetic fields. Here and following, the periodic boundary condition $\vec{\sigma}_{N+1}=\vec{\sigma}_1$ is assumed.

Now, we consider the FB grading. In the spin sector, the transfer matrix is constructed as Eq. (40) by the scattering matrix, Eq. (37). Taking the derivative of the logarithms of the transfer matrix, Eq. (40), with respect to the spin rapidity λ, we obtain the effective Hamiltonian of the system in the strong-coupling limit with the FB grading

$$H=-\frac{1}{2}\sum_{j=1}^{N}(\sigma_j^x\sigma_{j+1}^x+\sigma_j^y\sigma_{j+1}^y-2\sigma_j^z). \tag{112}$$

It is the 1D XY model with transverse magnetic fields.

The spin operators can be expressed by the bosonic or fermionic creation and annihilation operators with internal degree of freedom. The internal degree of freedom corresponds to the components. The exact relations between the spin operators and the creation and annihilation operators are

$$\sigma_j^x=c_{j\uparrow}^\dagger c_{j\downarrow}+c_{j\downarrow}^\dagger c_{j\uparrow},$$

$$\sigma_j^y = -i(c_{j\uparrow}^\dagger c_{j\downarrow} - c_{j\downarrow}^\dagger c_{j\uparrow}),$$

$$\sigma_j^z = n_{j\uparrow} - n_{j\downarrow}, \tag{113}$$

where $n_{js}=c_{js}^\dagger c_{js}$ $(s=\uparrow,\downarrow)$ is the particle number operator. Staring from above relations and using the Schriffer-Wolf transformation, we also obtain the effective Hamiltonians (121) and (124) with a global coefficient $t^2/(2U)$. These results are consistent with that obtained in Ref. 80.

VII. OTHER GRADINGS

The graded quantum inverse scattering method used in this paper still have two cases. One is the bosonic-bosonic (BB) grading, which corresponds the two-component bosons in the 1D optical lattice or the SU(2) Bose-Hubbard model. The other is the fermionic-fermionic (FF) grading, which corresponds the two-component fermions in the 1D optical lattice or the Fermi-Hubbard model.

A. Case I: Two-component bosons in 1D optical lattice

In the BB grading, $\epsilon_1=\epsilon_2=0$. This method is valid for the 1D lattice model of SU(2) bosons. The Hamiltonian is still quantified by Eq. (1) with the changing of all the spinless fermions by the another species of bosons. The permutation operator in this case is $[P_{\rm BB}]_{\alpha\mu}^{\beta\nu}=\delta_{\alpha\nu}\delta_{\mu\beta}$. Using the standing algebraic Bethe ansatz, we obtain the following commutation relations,

$$A(\lambda)C(u) = \frac{a(\lambda-u)-b(\lambda-u)}{a(\lambda-u)}C(u)A(\lambda) + \frac{b(\lambda-u)}{a(\lambda-u)}C(\lambda)D(u), \tag{114}$$

$$D(\lambda)C(u) = \frac{a(u-\lambda)-b(u-\lambda)}{a(u-\lambda)}C(u)D(\lambda) + \frac{b(u-\lambda)}{a(u-\lambda)}C(\lambda)D(u), \tag{115}$$

$$C(\lambda)C(u) = C(u)C(\lambda). \tag{116}$$

The elements $C(\lambda)$ and $C(u)$ commute with each other. The Bethe ansatz equations are

$$e^{ik_jL} = \prod_{l=1}^{N} \frac{\sin k_j - \sin k_l + i\frac{U}{2}}{\sin k_j - \sin k_l - i\frac{U}{2}} \times \prod_{\alpha=1}^{M} \frac{\sin k_j - \lambda_\alpha - i\frac{U}{4}}{\sin k_j - \lambda_\alpha + i\frac{U}{4}}, \quad j=1,\ldots,N, \tag{117}$$

$$\prod_{l=1}^{N} \frac{\lambda_\beta - \sin k_l - i\frac{U}{4}}{\lambda_\beta - \sin k_l + i\frac{U}{4}} = \prod_{\gamma\neq\beta}^{M} \frac{\lambda_\beta - \lambda_\gamma - i\frac{U}{2}}{\lambda_\beta - \lambda_\gamma + i\frac{U}{2}}, \tag{118}$$

where $\beta=1,\ldots,M$, $N=N_{b_1}+N_{b_2}$, and $M=N_{b_2}$. Taking the logarithm of Eqs. (117) and (118), we arrive at

$$k_jL = 2\pi I_j - 2\sum_{l=1}^{N} \theta_{1/2}(\sin k_j - \sin k_l) + 2\sum_{\alpha=1}^{M} \theta_{1/4}(\sin k_j - \lambda_\alpha),$$

$$\pi J_\beta = \sum_{l=1}^{N} \theta_{1/4}(\lambda_\beta - \sin k_l) - \sum_{\alpha=1}^{M} \theta_{1/2}(\lambda_\beta - \lambda_\alpha).$$

Here the quantum numbers I_j and J_β take integer or half-odd integer values, depending on whether N and M are even or odd, respectively. The energy E and the momentum P are

$$E = -2\sum_{j=1}^{N} \cos k_j, \quad P = \sum_{j=1}^{N} k_j. \tag{119}$$

In the thermodynamic limit, the densities of state satisfy following integration equations

$$\rho(k) = \frac{1}{2\pi} + \frac{\cos k}{\pi}\int_{-Q}^{Q} \frac{2U\rho(k')dk'}{U^2+4(\sin k - \sin k')^2} - \frac{1}{\pi}\int_{-B}^{B} \frac{4U\sigma(\lambda)d\lambda}{U^2+16(\sin k-\lambda)^2}, \tag{120}$$

$$\sigma(\lambda) = \frac{1}{\pi}\int_{-Q}^{Q} \frac{4U\rho(k)dk}{U^2+16(\lambda-\sin k)^2} - \frac{1}{\pi}\int_{-B}^{B} \frac{2U\sigma(\lambda')d\lambda'}{U^2+4(\lambda-\lambda')^2}. \tag{121}$$

The integral limits Q and B are determined by $N/L=\int_{-Q}^{Q}\rho(k)dk$ and $M/L=\int_{-B}^{B}\sigma(\lambda)d\lambda$. The densities of energy and momentum are $E/L=-2t\int_{-Q}^{Q}\cos k\rho(k)dk$ and $P/L=\int_{-Q}^{Q}k\rho(k)dk$, respectively.

In the strong-coupling limit, the effective Hamiltonian reads

$$H = -\frac{1}{2}\sum_{j=1}^{N} \vec{\sigma}_j \cdot \vec{\sigma}_{j+1}. \tag{122}$$

It is the ferromagnetic isotropic Heisenberg model.

B. Case II: Two-component fermions in 1D optical lattice

In the FF grading, $\epsilon_1=\epsilon_2=1$. The method is valid for the two-component fermions in the 1D optical lattice or the spin-1/2 Fermi-Hubbard model. The Pauli exclusive principle requires that two fermions belong to the same species can not occupy the same position. Thus the integrability is satisfied naturally. The system is SU(2) invariant. The permutation operator in this case is $[P_{\rm FF}]_{\alpha\mu}^{\beta\nu}=-\delta_{\alpha\nu}\delta_{\mu\beta}$. The two-body scattering matrix satisfies the Yang-Baxter equations. From it, we obtain following commutation relations,

$$A(\lambda)C(u) = \frac{1}{a(\lambda-u)}C(u)A(\lambda) - \frac{b(\lambda-u)}{a(\lambda-u)}C(\lambda)D(u),$$

$$D(\lambda)C(u) = \frac{1}{a(u-\lambda)}C(u)D(\lambda) - \frac{b(u-\lambda)}{a(u-\lambda)}C(\lambda)D(u),$$

$$C(\lambda)C(u) = C(u)C(\lambda).$$

Using the standing Bethe ansatz method, one can obtain the Bethe ansatz equations as[43,81]

$$e^{ik_jL} = \prod_{\alpha=1}^{N_b} \frac{\sin k_j - \lambda_\alpha + i\frac{U}{4}}{\sin k_j - \lambda_\alpha - i\frac{U}{4}}, \tag{123}$$

$$\prod_{l=1}^{N} \frac{\lambda_\beta - \sin k_l - i\frac{U}{4}}{\lambda_\beta - \sin k_l + i\frac{U}{4}} = \prod_{\gamma\neq\beta}^{M} \frac{\lambda_\beta - \lambda_\gamma - i\frac{U}{2}}{\lambda_\beta - \lambda_\gamma + i\frac{U}{2}}, \tag{124}$$

where $j=1,\ldots,N$, $\beta=1,\ldots,M$, $N=N_{f_1}+N_{f_2}$, and $M=N_{f_2}$. The Fermi-Hubbard model has many applications in the low-dimensional strongly correlated system, superconductivity theory and other aspects of the condensed-matter physics. The exact solutions and Mott-insulator phase transition have been studied by Lieb and Wu[43] and the thermodynamic properties have been studied by Takahashi.[81] In the strong-coupling limit, the effective Hamiltonian is

$$H = \frac{1}{2}\sum_{j=1}^{N} \vec{\sigma}_j \cdot \vec{\sigma}_{j+1}. \tag{125}$$

It is the antiferromagnetic isotropic Heisenberg model.

VIII. CONCLUSIONS

In summary, we study the mixture of scalar bosons and polarized fermions in the 1D optical lattice. The system is modeled by the Bose-Fermi-Hubbard Hamiltonian, which shows different behavior from that of the Bose-Hubbard or the Fermi-Hubbard models. There exists a critical on-site interaction U_c. If $U<U_c$, the ground state of the system is in the superfluid phase, while if $U>U_c$, the ground state is in the insulating phase. The superfluid-insulator transition occurs at U_c. From the analysis of the superfluid density, we obtain the value of the critical point as $U_c=2.79256\pm0.00112$, which is larger than the $U_c=0$ for the Fermi-Hubbard model and smaller than the $U_c=3.28$ for the Bose-Hubbard model. The elementary excitations, strong-coupling limit and effective Hamiltonian are also discussed.

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