

Exact solution of the extended dimer Bose–Hubbard model with multi-body interactions

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Abstract. It is shown that the extended one-dimensional dimer Bose–Hubbard model with multi-body interactions can be solved exactly by using the algebraic Bethe ansatz mainly due to the site-permutation S_2 symmetry. The solution for the model with up to three-particle hopping and three-body on-site interaction is explicitly shown. As an example of the application, lower part of the excitation energy levels and the ground-state entanglement measure of the standard Bose–Hubbard Hamiltonian with the attractive two-body on-site interaction plus the three-body on-site interaction for 100 bosons with variation of the control parameter are calculated by using the exact solution. It is shown that the attractive three-body on-site interaction reinforces the critical point entanglement of the system, which may be helpful for design of an optical lattice for ultracold atoms or a tuneable superconducting quantum interference device with maximal entanglement.

Keywords: algebraic structures of integrable models, Bose Einstein condensation, Hubbard and related model, quantum integrability (Bethe Ansatz)

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1. Introduction

The behavior of interacting bosonic many-body systems has been of great interests since they capture a wide variety of physical problems [1, 2]. The standard Bose–Hubbard model is the simplest theory that can be used to model the main features in these strongly interacting bosonic systems [3]. Up till now, the scope of the Bose–Hubbard model has been extended to include the effects of excited bands, long-range interactions and density-induced tunnelings [4]. Much progress in the extended Bose–Hubbard model (EBHM) with up to two-particle hopping and two-body on-site interaction has been made both theoretically and experimentally [5]. Moreover, it has been shown that the EBHM with effective multi-body interactions may be more appropriate in some cases, and can give rise to novel quantum phases with intriguing properties [6–10]. For example, polar molecules in optical lattices driven by microwave fields give naturally rise to Hubbard models with strong nearest-neighbor three-body interactions [7]. It is shown in [8] that the two-band BH Hamiltonian over a wide range of lattice parameters is equivalent to an effective single-band Hamiltonian with strong three-body interactions. Three-body loss of atoms in an optical lattice can also give rise to effective hard-core three-body interactions. In [10–12], the phase diagram of the extended Bose–Hubbard model with two- and three-body on-site interactions was studied by directly diagonalizing the matrix of the Hamiltonian in the Fock subspace, the mean-field approximation, and the density matrix renormalization group method.

On the other hand, small systems with a few sites are also of interests since they are extremely relevant to bond excitations in small molecules [13] and BECs in optical traps with a few wells [14], which can be realized experimentally with microtrap technology [15]. The two-site (dimer) system, which can be used to describe the Josephson effect in superconducting qubits [16, 17], nonlinear self-trapping of Bose–Einstein condensates [18], and fermionic mixtures [19], has been analyzed thoroughly from both the semi-classical [20] and purely quantum viewpoint [16, 21, 22]. Recently, it has been shown in

[9] that an effective two-mode model with the three-body interaction and a three-body interaction-induced tunneling term can be used to describe the low-energy physics of bosons in a double-well potential with a high barrier between the wells and sufficiently weak atom–atom interactions. Moreover, it has been shown that the Bose–Hubbard model and the EBHM with up to two-body interactions for dimer case can be solved exactly by using the algebraic Bethe ansatz [23], which are equivalent to special cases of the LMG model after the $SU(2)$ realization whose exact solution was provided in [24]. As shown in the previous work [25], the roots of the Bethe ansatz equations of the dimer Bose–Hubbard model are zeros of the one-variable extended Heine–Stieltjes polynomials, which can be determined more easily than directly solving the BAEs with a set of variables. Since there are only two degrees of freedom in both particle-number conserving bipartite fermion and boson systems, the dimer Bose–Hubbard model and other similar particle-number conserving bipartite quantum systems with multi-body interactions should always be exactly solvable due to the fact that there are two constants of motion of the system, namely the Hamiltonian itself and the total number of particles. However, a rigorous and explicit proof of its exact solvability is lacking.

In this work, it is shown that the one-dimensional EBHM with multi-body interactions for dimer case can be solved exactly due to the site-permutation S_2 symmetry, though, in the following, the procedure is demonstrated for the model with up to three-particle hopping and three-body on-site interaction only.

2. Solution of the model

The Hamiltonian of the one-dimensional dimer EBHM with multi-body interactions may be expressed as [5–10]

$$\hat{H} = t\hat{N} - t\hat{H}_1 + \sum_{q \geq 2} U_q \hat{H}_{q,1} + \sum_{q \geq 2} t_q \hat{H}_{q,2}, \quad (1)$$

where $\hat{N} = \hat{n}_1 + \hat{n}_2$, $\hat{H}_1 = (a_1^\dagger + a_2^\dagger)(a_1 + a_2)$, $\hat{H}_{q,1} = \sum_{i=1}^2 \hat{n}_i^q$, $\hat{H}_{q,2} = a_1^{\dagger q} a_2^q + a_2^{\dagger q} a_1^q$, t , t_q are the effective single-, q -particle hopping parameters, respectively, and U_q are the effective q -body on-site interaction parameters, in which a_i (a_i^\dagger) are boson annihilation (creation) operators obeying the canonical commutation relations $[a_i, a_j^\dagger] = \delta_{ij}$, and $\hat{n}_i = a_i^\dagger a_i$ is the boson number operator at site i . It is obvious that the Hamiltonian of the standard dimer Bose–Hubbard model [3] or the dimer EBHM with up to two-body interactions [5] is a special case of (1).

The Hamiltonian (1) clearly commutes with the total number of bosons \hat{N} in the system. Therefore, for a given number of bosons, N , the Hamiltonian (1) can be diagonalized in the Fock subspace V_N spanned by $\{a_1^{\dagger N-n} a_2^{\dagger n} |0\rangle\}$ with $n = 0, 1, 2, \dots, N$, where $|0\rangle$ is the boson vacuum state, of which the dimension is just equal to that of the symmetric irrep $[N, 0]$ of $U(2)$ with $\dim(V_N) = N + 1$. Furthermore, the Hamiltonian (1) is invariant under the S_2 site-permutation. Hence, the Hamiltonian (1) under the Fock subspace V_N can be block diagonalized according to two different types of irreducible representations of S_2 , of which the subspaces are denoted as V_S and V_A for the

symmetric and anti-symmetric one, respectively. In general, according to the theory of symmetric functions [26], basis vectors of the symmetric subspace V_S may be expanded in terms of products of powers of the elementary symmetric polynomials of the boson creation operators. For the dimer case, there are only two independent symmetric polynomials, the collective boson operator $S_1^\dagger = a_1^\dagger + a_2^\dagger$ and boson-pair operator $S_2^\dagger = a_1^\dagger a_2^\dagger$, and one elementary antisymmetric operator $A^\dagger = a_1^\dagger - a_2^\dagger$. Therefore, V_S is spanned by $\{S_1^{\dagger N-2r} S_2^{\dagger r} |0\rangle\}$, while V_A is spanned by $\{S_1^{\dagger N-2r} S_2^{\dagger r} A^\dagger |0\rangle\}$ with $r = 0, 1, 2, \dots, [N/2]$, where $[x]$ denotes the integer part of x , because any homogeneous two-variable antisymmetric polynomial can always be expressed as product of a homogeneous symmetric polynomial times the elementary antisymmetric binomial A^\dagger .

Using the bosonic commutation relations among $\{a_i, a_i^\dagger\}$, we have $[S_1, S_1^\dagger] = 2$, $[S_2, S_2^\dagger] = \hat{N} + 1$, $[S_1, S_2^\dagger] = S_1^\dagger$, $[S_1, A^\dagger] = 0$, $[S_2, A^\dagger] = -A$, and $[A, A^\dagger] = 2$. One can easily check that the commutator $[H_1, S^\dagger]$ with $S^\dagger = S_1^\dagger$ or S_2^\dagger results in monomials of S_1^\dagger . Though the commutator $[\hat{H}_{q,p}, S^\dagger]$ results in new operators related to the local boson number operators, the direct operation of $[\hat{H}_{q,p}, S^\dagger]$ to the vacuum state always results in a polynomial of S_1^\dagger and S_2^\dagger . Similarly, the direct operation of μ -time commutator $[\dots [H_{q,p}, S^\dagger], \dots], S^\dagger]$ to the vacuum state also results in a polynomial of S_1^\dagger and S_2^\dagger , which may be nonzero only when $\mu \leq q$. As the consequence, the operation of the Hamiltonian (1) to $G_1(S_1^\dagger, S_2^\dagger)|0\rangle$, where $G_1(S_1^\dagger, S_2^\dagger)$ is a homogeneous polynomial in S_1^\dagger and S_2^\dagger on complex field, results in $G_2(S_1^\dagger, S_2^\dagger)|0\rangle$, where $G_2(S_1^\dagger, S_2^\dagger)$ is also a homogeneous polynomial in S_1^\dagger and S_2^\dagger of the same degree on complex field. Therefore, the operation of the Hamiltonian (1) to $\{G_\mu(S_1^\dagger, S_2^\dagger)|0\rangle\}$, where $\{G_\mu(S_1^\dagger, S_2^\dagger)\}$ is the homogeneous polynomial ring, is algebraically closed. Similarly, the operation of the Hamiltonian (1) to any state vector in V_A is also within V_A . Furthermore, any two-variable homogeneous polynomials in $S_1^{\dagger 2}$ and S_2^\dagger on complex field can always be expressed as products of binomials. Hence, similar to the Bethe ansatz used for solving the standard Bose–Hubbard model and the EBHM with up to two-body interactions, up to a normalization constant, eigen-states of (1) within the symmetric subspace V_S can be expressed as

$$|N, \zeta\rangle_S = \begin{cases} \prod_{\rho=1}^k S^\dagger(x_\rho^{(\zeta)})|0\rangle & \text{for } N = 2k, \\ \prod_{\rho=1}^k S^\dagger(x_\rho^{(\zeta)})S_1^\dagger|0\rangle & \text{for } N = 2k + 1, \end{cases} \quad (2)$$

where $S^\dagger(x) = xS_2^\dagger + S_1^{\dagger 2}$ is a binomial of $S_1^{\dagger 2}$ and S_2^\dagger , in which x is a complex parameter to be determined, and ζ labels the ζ -th eigen-vector of (1). Similarly, eigen-states of (1) within the antisymmetric subspace V_A may be expressed as

$$|N, \zeta\rangle_A = \begin{cases} \prod_{\rho=1}^k S^\dagger(x_\rho^{(\zeta)})S_1^\dagger A^\dagger|0\rangle & \text{for } N = 2k + 2, \\ \prod_{\rho=1}^k S^\dagger(x_\rho^{(\zeta)})A^\dagger|0\rangle & \text{for } N = 2k + 1. \end{cases} \quad (3)$$

It is obvious that there are $k + 1$ independent terms when (2) and (3) are expanded in terms of $S_1^{\dagger 2}$ and S_2^{\dagger} for either $N = 2k$ or $N = 2k + 1$ case. Therefore, the number of independent eigenvectors shown in (2) and (3) for any N equals exactly to $\dim(V_N)$. It should be stated that (2) and (3) is of the Bethe vector form similar to that used for the standard Bose–Hubbard model case [27], which is useful in the planar $\mathcal{N} = 4$ super Yang–Mills theory [28] in the context of the integrability under the AdS/CFT correspondence [29].

In order to prove that the Bethe vector states shown in (2) and (3) are indeed the eigen-states of (1), the commutation relations of each term in (1) with $S^{\dagger}(x_i)$, S^{\dagger} , and A^{\dagger} are useful. It is obvious that only the single-commutators need to be calculated for the one-body term \hat{H}_1 , because $[\hat{H}_1, \hat{O}^{\dagger}]$, where O^{\dagger} may be taken as $S^{\dagger}(x_i)$, S^{\dagger} , or A^{\dagger} , is commutative with any other operator involved in (2) or (3). Similarly, only the μ -time commutators $[\dots [\hat{H}_{q,p}, \hat{O}^{\dagger}], \dots], \hat{O}^{\dagger}]$ for $\mu = 1, \dots, q$ need to be calculated. Once these commutators are obtained, the vacuum valued polynomial $G(S_1^{\dagger}, S_2^{\dagger})$ in S_1^{\dagger} and S_2^{\dagger} defined as $G(S_1^{\dagger}, S_2^{\dagger})|0\rangle \equiv [\dots [\hat{H}_{q,p}, \hat{O}^{\dagger}], \dots], \hat{O}^{\dagger}] |0\rangle$ are needed, where $[\dots [\hat{H}_{q,p}, \hat{O}^{\dagger}], \dots], \hat{O}^{\dagger}]$ is the μ -time commutator with $\mu \leq q$. As an example of the exact solution, the vacuum valued nonzero commutators useful for the Hamiltonian with up to three-body interactions ($q \leq 3$) are shown in tables 1–3, in which

$$\begin{aligned}
 F_{2,1}^{(e)}(x_1; x_2) &= \frac{4x_1 + 16}{x_1 - x_2}, \\
 F_{2,2}^{(e)}(x_1; x_2) &= \frac{2(x_1 + 4)(x_1x_2 + 2x_1 + 2x_2 + 2)}{x_1 - x_2}, \\
 F_{3,1}^{(e)}(x_1; x_2) &= \frac{6(3x_1(x_1 + 6) - (x_1 + 2)x_2)}{x_1(x_1 - x_2)}, \\
 F_{3,2}^{(e)}(x_1; x_2) &= \frac{6(x_1^3 + 8x_1^2 + 14x_1 + (x_1^2 + 4x_1 + 2)x_2)}{x_1(x_1 - x_2)}, \\
 V_{3,1}^{(e)}(x_1; x_2, x_3) &= \frac{12(x_1 + 4)(2x_1 - x_2 - x_3)}{(x_1 - x_2)(x_1 - x_3)}, \\
 V_{3,2}^{(e)}(x_1; x_2, x_3) &= 6(x_1 + 4) \frac{4x_1(x_1 + 2) + 2(x_1^2 + 3x_1 + 1)(x_2 + x_3) + (x_1 + 1)(x_1 + 3)x_2x_3}{(x_1 - x_2)(x_1 - x_3)}, \\
 F_{3,1}^{(o)}(x_1; x_2) &= \frac{6(x_1 - 2x_2)(4 + x_2)}{(x_1 - x_2)x_2}, \\
 F_{3,2}^{(o)}(x_1; x_2) &= \frac{6(x_1 + 4)(2x_1(x_1 + 2) + (x_1^2 + 3x_1 + 1)x_2)}{x_1(x_1 - x_2)}, \\
 F_{3,1}^{(A)}(x_1; x_2) &= \frac{6(x_1 - 2(x_2 + 2))}{x_1 - x_2}, \\
 F_{3,2}^{(A)}(x_1; x_2) &= -\frac{6(2x_1^2 + 8x_1 + 4 + (x_1^2 + 5x_1 + 5)x_2)}{x_1 - x_2}. \tag{4}
 \end{aligned}$$

Table 1. Vacuum valued nonzero commutators $[\dots [\hat{H}_{q,p}, S^\dagger(x_1)], \dots, S^\dagger(x_{k-1})], S^\dagger(x_k)] |0\rangle$ for $q \leq 3$ and $k \leq 3$.

	$S^\dagger(x)$	$S_1^{\dagger 2}$		
$[\hat{H}_1, S^\dagger(x)]$	0	$x + 4$		
$[\hat{H}_{2,1}, S^\dagger(x)]$	$\frac{2x-4}{x}$	$\frac{2x+4}{x}$		
$[\hat{H}_{2,2}, S^\dagger(x)]$	$-\frac{4}{x}$	$\frac{2x+4}{x}$		
$[\hat{H}_{3,1}, S^\dagger(x)]$	$\frac{2x-12}{x}$	$\frac{6x+12}{x}$		
	$S^\dagger(x_1)S^\dagger(x_2)$	$S^\dagger(x_1)S_1^{\dagger 2}$	$S^\dagger(x_2)S_1^{\dagger 2}$	
$[\hat{H}_{2,1}, S^\dagger(x_1)], S^\dagger(x_2)]$	4	$F_{2,1}^{(e)}(x_2; x_1)$	$F_{2,1}^{(e)}(x_1; x_2)$	
$[\hat{H}_{2,2}, S^\dagger(x_1)], S^\dagger(x_2)]$	4	$F_{2,2}^{(e)}(x_2; x_1)$	$F_{2,2}^{(e)}(x_1; x_2)$	
$[\hat{H}_{3,1}, S^\dagger(x_1)], S^\dagger(x_2)]$	$12 - \frac{12}{x_1} - \frac{12}{x_2}$	$F_{3,1}^{(e)}(x_2; x_1)$	$F_{3,1}^{(e)}(x_1; x_2)$	
$[\hat{H}_{3,2}, S^\dagger(x_1)], S^\dagger(x_2)]$	$\frac{12}{x_1} + \frac{12}{x_2}$	$F_{3,2}^{(e)}(x_2; x_1)$	$F_{3,2}^{(e)}(x_1; x_2)$	
	$S^\dagger(x_1)S^\dagger(x_2)S^\dagger(x_3)$	$S^\dagger(x_1)S^\dagger(x_2)S_1^{\dagger 2}$	$S^\dagger(x_1)S_1^{\dagger 2}S^\dagger(x_3)$	$S_1^{\dagger 2}S^\dagger(x_2)S^\dagger(x_3)$
$[\hat{H}_{3,1}, S^\dagger(x_1)], S^\dagger(x_2)], S^\dagger(x_3)]$	12	$V_{3,1}^{(e)}(x_3; x_1, x_2)$	$V_{3,1}^{(e)}(x_2; x_1, x_3)$	$V_{3,1}^{(e)}(x_1; x_2, x_3)$
$[\hat{H}_{3,2}, S^\dagger(x_1)], S^\dagger(x_2)], S^\dagger(x_3)]$	-12	$V_{3,2}^{(e)}(x_3; x_1, x_2)$	$V_{3,2}^{(e)}(x_2; x_1, x_3)$	$V_{3,2}^{(e)}(x_1; x_2, x_3)$

As shown in tables 1–3, these vacuum valued commutators involving k operators $S^\dagger(x_i)$ for $i = 1, \dots, k$ result in $k + 1$ terms, of which one is proportional to the original operator product $\prod_{i=1}^k S^\dagger(x_i)$, and other k terms are proportional to $\prod_{i \neq j}^k S^\dagger(x_i)S_1^{\dagger 2}$ for $j = 1, \dots, k$. As the consequence, if (2) or (3) is the eigen-state of (1), the coefficient of proportionality of (2) or (3) after the operation of (1) to (2) or (3) gives the eigenvalue of (1) equivalent to the eigen-equation $\hat{H}|N, \zeta\rangle = E_N^{(\zeta)}|N, \zeta\rangle$, while the other k terms proportional to $\prod_{i \neq j}^k S^\dagger(x_i)S_1^{\dagger 2}$ for $j = 1, \dots, k$ must be zero, which, thus, leads to the Bethe ansatz equations in determining the k variables $\{x_1, \dots, x_k\}$. Accordingly, when $q \leq 3$, the eigen-energy of (1) within the symmetric subspace is

$$E_N^{(\zeta), S} = \delta_{N, 2k+1} E_N^{(\zeta), o} + k(2U_3 k^2 + 2U_2 k - t_3(k-1)(k-2) + 2t_2(k-1) + 2t) + (12(t_3 - U_3)k - 4t_2 - 12t_3 - 4U_2) \sum_{i=1}^k \frac{1}{x_i^{(\zeta)}}, \quad (5)$$

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Table 2. Vacuum valued nonzero commutators $[\dots[\hat{H}_{q,p}, S^\dagger(x_1)], \dots, S^\dagger(x_{k-1})], S_1^\dagger |0\rangle$ for $q \leq 3$ and $k \leq 3$. The other three are $[\hat{H}_1, S_1^\dagger]|0\rangle = 2S_1^\dagger|0\rangle$, $[\hat{H}_{2,1}, S_1^\dagger]|0\rangle = [\hat{H}_{3,1}, S_1^\dagger]|0\rangle = S_1^\dagger|0\rangle$.

	$S^\dagger(x)S_1^\dagger$	$S_1^{\dagger 3}$	
$[[\hat{H}_{2,1}, S^\dagger(x)], S_1^\dagger]$	$\frac{2x-8}{x}$	$\frac{2x+8}{x}$	
$[\hat{H}_{2,2}, S^\dagger(x), S_1^\dagger]$	$-\frac{6x+8}{x}$	$\frac{2(x+1)(x+4)}{x}$	
$[\hat{H}_{3,1}, S^\dagger(x), S_1^\dagger]$	$\frac{6x-42}{x}$	$\frac{12x+42}{x}$	
$[\hat{H}_{3,2}, S^\dagger(x), S_1^\dagger]$	$-\frac{18}{x}$	$\frac{6x+18}{x}$	
	$S^\dagger(x_1)S^\dagger(x_2)S_1^\dagger$	$S^\dagger(x_1)S_1^{\dagger 3}$	$S_1^{\dagger 2}S^\dagger(x_2)S_1^\dagger$
$[[\hat{H}_{3,1}, S^\dagger(x_1)], S^\dagger(x_2)], S_1^\dagger]$	$6 - \frac{24}{x_1} - \frac{24}{x_2}$	$F_{3,1}^{(o)}(x_2; x_1)$	$F_{3,1}^{(o)}(x_1; x_2)$
$[[\hat{H}_{3,2}, S^\dagger(x_1)], S^\dagger(x_2)], S_1^\dagger]$	$30 + \frac{24}{x_1} + \frac{24}{x_2}$	$F_{3,2}^{(o)}(x_2; x_1)$	$F_{3,2}^{(o)}(x_1; x_2)$

Table 3. Vacuum valued nonzero commutators $[[\hat{H}_{q,p}, S^\dagger(x)], A^\dagger]|0\rangle$, $[[[\hat{H}_{q,p}, S^\dagger(x)], S_1^\dagger], A^\dagger]|0\rangle$, and $[[[\hat{H}_{q,p}, S^\dagger(x_1)], S^\dagger(x_2)], A^\dagger]|0\rangle$ for $q \leq 3$. The other ones are $[\hat{H}_{2,1}, A^\dagger]|0\rangle = [\hat{H}_{3,1}, A^\dagger]|0\rangle = A^\dagger|0\rangle$, $[\hat{H}_{2,1}, S_1^\dagger], A^\dagger |0\rangle = -[\hat{H}_{2,2}, S_1^\dagger], A^\dagger |0\rangle = 2S_1^\dagger A^\dagger|0\rangle$, and $[\hat{H}_{3,1}, S_1^\dagger], A^\dagger |0\rangle = 6S_1^\dagger A^\dagger|0\rangle$.

	$S^\dagger(x)A^\dagger$	$S_1^{\dagger 2}A^\dagger$	
$[[\hat{H}_{2,1}, S^\dagger(x)], A^\dagger]$	2	2	
$[[\hat{H}_{2,2}, S^\dagger(x)], A^\dagger]$	2	$-(2x+6)$	
$[[\hat{H}_{3,1}, S^\dagger(x)], A^\dagger]$	$\frac{6x-6}{x}$	$\frac{12x+6}{x}$	
$[[\hat{H}_{3,2}, S^\dagger(x)], A^\dagger]$	$\frac{6}{x}$	$-\frac{6x+6}{x}$	
	$S^\dagger(x)S_1^\dagger A^\dagger$	$S_1^{\dagger 3}A^\dagger$	
$[[[\hat{H}_{3,1}, S^\dagger(x)], S_1^\dagger], A^\dagger]$	$\frac{6x-12}{x}$	$\frac{6x+12}{x}$	
$[[[\hat{H}_{3,2}, S^\dagger(x)], S_1^\dagger], A^\dagger]$	$\frac{12x+12}{x}$	$-\frac{6(x^2+4x+2)}{x}$	
	$S^\dagger(x_1)S^\dagger(x_2)A^\dagger$	$S^\dagger(x_1)S_1^{\dagger 2}A^\dagger$	$S_1^{\dagger 2}S^\dagger(x_2)A^\dagger$
$[[\hat{H}_{3,1}, S^\dagger(x_1)], S^\dagger(x_2)], A^\dagger]$	6	$F_{3,1}^{(A)}(x_2; x_1)$	$F_{3,1}^{(A)}(x_1; x_2)$
$[[\hat{H}_{3,2}, S^\dagger(x_1)], S^\dagger(x_2)], A^\dagger]$	-6	$F_{3,2}^{(A)}(x_2; x_1)$	$F_{3,2}^{(A)}(x_1; x_2)$

where

$$E_N^{(\zeta),o} = k(3(U_3 + 5t_3)k + 2U_2 - 15t_3 - 6t_2 + 3U_3) + U_2 + U_3 - 2t + (24(t_3 - U_3)k - 8U_2 - 8t_2 - 18U_3 - 42t_3) \sum_{i=1}^k \frac{1}{x_i^{(\zeta)}} \quad (6)$$

for $N = 2k$ or $N = 2k + 1$, in which the k variables $\{x_1^{(\zeta)}, \dots, x_k^{(\zeta)}\}$ should satisfy

$$\begin{aligned} & -t(x_i^{(\zeta)} + 4) + (U_2 + t_2) \frac{2x_i^{(\zeta)} + 4}{x_i^{(\zeta)}} + U_3 \frac{2x_i^{(\zeta)} + 12}{x_i^{(\zeta)}} + \sum_{j(\neq i)} \sum_{q=2}^3 \left(U_q F_{q,1}^{(e)}(x_i^{(\zeta)}; x_j^{(\zeta)}) \right. \\ & \left. + t_q F_{q,2}^{(e)}(x_i^{(\zeta)}; x_j^{(\zeta)}) \right) + \delta_{N,2k+1} \left(U_2 \frac{2x_i^{(\zeta)} + 8}{x_i^{(\zeta)}} + 2t_2 \frac{(x_i^{(\zeta)} + 1)(x_i^{(\zeta)} + 4)}{x_i^{(\zeta)}} \right. \\ & \left. + U_3 \frac{12x_i^{(\zeta)} + 42}{x_i^{(\zeta)}} + t_3 \frac{6x_i^{(\zeta)} + 18}{x_i^{(\zeta)}} \right) + \delta_{N,2k+1} \sum_{j(\neq i)} \left(U_3 F_{3,1}^{(o)}(x_i^{(\zeta)}; x_j^{(\zeta)}) \right. \\ & \left. + t_3 F_{3,2}^{(o)}(x_i^{(\zeta)}; x_j^{(\zeta)}) \right) + \sum_{j \neq l(\neq i)} \left(U_3 V_{3,1}^{(e)}(x_i^{(\zeta)}; x_j^{(\zeta)}, x_l^{(\zeta)}) \right. \\ & \left. + t_3 V_{3,2}^{(e)}(x_i^{(\zeta)}; x_j^{(\zeta)}, x_l^{(\zeta)}) \right) = 0 \text{ for } i = 1, 2, \dots, k, \end{aligned} \quad (7)$$

where ζ used in (5) and (7) labels the ζ -th solution of (7). While the eigen-energy of (1) for $q \leq 3$ within the antisymmetric subspace is given by

$$\begin{aligned} E_N^{(\zeta),A} &= U_2 + U_3 + 2(U_2 + t_2)k + 3(U_3 - t_3)k(k - 1) + 6U_3k \\ &+ 6(t_3 - U_3) \sum_{i=1}^k \frac{1}{x_i^{(\zeta)}} + \delta_{N,2k+2} \left(E_N^{(\zeta),o} + 2(U_2 - t_2) + 6U_3 \right. \\ &+ 6(U_3 + 2t_3)k + 12(t_3 - U_3) \sum_{i=1}^k \frac{1}{x_i^{(\zeta)}} \left. \right) \\ &+ k(2U_3k^2 + 2U_2k - t_3(k - 1)(k - 2) + 2t_2(k - 1) + 2t) \\ &+ (12(t_3 - U_3)k - 4t_2 - 12t_3 - 4U_2) \sum_{i=1}^k \frac{1}{x_i^{(\zeta)}} \end{aligned}$$

for $N = 2k + 1$ or $N = 2k + 2$, in which the k variables $\{x_1^{(\zeta)}, \dots, x_k^{(\zeta)}\}$ should satisfy

$$\begin{aligned}
 & -t(x_i^{(\zeta)} + 4) + (U_2 + t_2) \frac{2x_i^{(\zeta)} + 4}{x_i^{(\zeta)}} + U_3 \frac{2x_i^{(\zeta)} + 12}{x_i^{(\zeta)}} + \sum_{j(\neq i)} \sum_{q=2}^3 \left(U_q F_{q,1}^{(e)}(x_i^{(\zeta)}; x_j^{(\zeta)}) \right. \\
 & \left. + t_q F_{q,2}^{(e)}(x_i^{(\zeta)}; x_j^{(\zeta)}) \right) + 2U_2 - t_2(2x_i^{(\zeta)} + 6) + U_3 \frac{12x_i^{(\zeta)} + 6}{x_i^{(\zeta)}} - t_3 \frac{6x_i^{(\zeta)} + 6}{x_i^{(\zeta)}} \\
 & + \sum_{j(\neq i)} \left(U_3 F_{3,1}^{(A)}(x_i^{(\zeta)}; x_j^{(\zeta)}) + t_3 F_{3,2}^{(A)}(x_i^{(\zeta)}; x_j^{(\zeta)}) \right) \\
 & + \sum_{j \neq l(\neq i)} \left(U_3 V_{3,1}^{(e)}(x_i^{(\zeta)}; x_j^{(\zeta)}, x_l^{(\zeta)}) + t_3 V_{3,2}^{(e)}(x_i^{(\zeta)}; x_j^{(\zeta)}, x_l^{(\zeta)}) \right) \\
 & + \delta_{N,2k+2} \left(U_2 \frac{2x_i^{(\zeta)} + 8}{x_i^{(\zeta)}} + 2t_2 \frac{(x_i^{(\zeta)} + 1)(x_i^{(\zeta)} + 4)}{x_i^{(\zeta)}} + U_3 \frac{12x_i^{(\zeta)} + 42}{x_i^{(\zeta)}} \right. \\
 & \left. + t_3 \frac{6x_i^{(\zeta)} + 18}{x_i^{(\zeta)}} \right) + \delta_{N,2k+2} \sum_{j(\neq i)} \left(U_3 F_{3,1}^{(o)}(x_i^{(\zeta)}; x_j^{(\zeta)}) + t_3 F_{3,2}^{(o)}(x_i^{(\zeta)}; x_j^{(\zeta)}) \right) \\
 & + \delta_{N,2k+2} \left(6U_3 \frac{x_i^{(\zeta)} + 2}{x_i^{(\zeta)}} - 6t_3 \frac{(x_i^{(\zeta)})^2 + 4x_i^{(\zeta)} + 2}{x_i^{(\zeta)}} \right) = 0 \text{ for } i = 1, 2, \dots, k. \quad (8)
 \end{aligned}$$

Once the ζ -th solution $\{x_1^{(\zeta)}, \dots, x_k^{(\zeta)}\}$ of (7) or (8) are obtained, the corresponding eigen-state (2) with $N = 2k$, for example, can be expressed as

$$|N, \zeta\rangle_S = \sum_{\mu=0}^k S^{(\mu)}(x_1, \dots, x_k) S_1^{\dagger 2k-2\mu} S_2^{\dagger \mu} |0\rangle, \quad (9)$$

where $S^{(\mu)}(x_1, \dots, x_k) = \sum_{1 \leq i_1 \leq \dots \leq i_\mu < k} \prod_{q=1}^{\mu} x_{i_q}$ is the μ -th elementary symmetric polynomial of the k root-components $\{x_1^{(\zeta)}, \dots, x_k^{(\zeta)}\}$ of (7), which is helpful for calculating matrix elements of physical quantities of the system.

3. Analysis of the model with three-body on-site interaction

To demonstrate the use of the exact solution, excited states and the corresponding energies of a special case of the model with variation of the parameters are calculated numerically and checked against the results obtained from the direct matrix diagonalization, of which the Hamiltonian is the original hopping with attractive two-body on-site interaction [22] plus a three-body on-site interaction [10–12]. This scenario is similar to the low-energy bosons in a double well potential with high barrier between the wells with weak atom–atom interactions described in [9], and considered in [10–12]. To study how the three-body term affects the transitional patterns of the system, the parameters

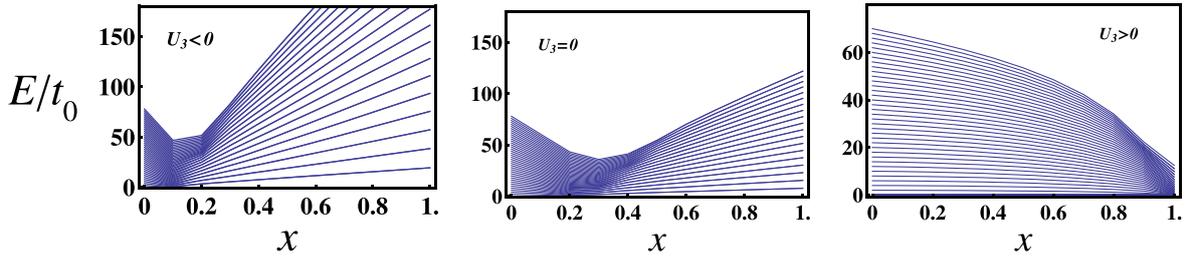


Figure 1. Some low-lying level energies [in unit of t_0 defined in (10)] of the two-site Bose–Hubbard model with attractive two-body on-site interaction and three-body on-site interaction with $U_3 < 0$, $U_3 = 0$, and $U_3 > 0$, respectively, as functions of x for $N = 100$ bosons.

of the Hamiltonian (1) for this case is reparameterized as

$$t = (1 - x)t_0, \quad U_2 = -4xt_0/(N + 1), \quad U_3 = \pm 4xt_0/(N + 1)^2, \quad (10)$$

where t_0 is a constant in arbitrary unit of energy and $x \in [0, 1]$. As is shown in the original model with $U_3 = 0$, the system is in the Fock regime when $x = 1$, in the Rabi regime when $x = 0$, and in the Josephson regime when $0 < x < 1$. Therefore, the solution of the model with variation of the control parameter $0 < x < 1$ can be used to study the quantum phase transitional behavior of the system in presence of the three-body on-site interaction. Figure 1 shows some low-lying level energies [in unit of t_0 defined in (10)] of the system with $x \in [0, 1]$ for $N = 100$ bosons, where no level-crossing occurs in the all cases concerned, especially at the ground state of the system. It is clearly shown in figure 1 that there is a minimum in the excitation energies around $x \sim 0.25$ – 0.35 with the highest energy level density which corresponds to the Josephson critical region when $U_3 = 0$. For $U_3 < 0$, the level pattern keeps similar to that in the $U_3 = 0$ case, of which the Josephson critical region is much narrower with a much deeper valley. It is obvious that the attractive three-body on-site interaction enhances the criticality in this case. In addition, the position of the minimum in the excitation energies shifts to a smaller x region with $x \sim 0.12$ – 0.18 when $U_3 < 0$. For $U_3 > 0$, the position with denser levels that are lower in energy shifts to a narrow region with $x \sim 0.93$ – 1.0 . In this case, the system almost keeps in the superfluid phase for $0 \leq x \leq x_c$ with $x_c \sim 0.92$, and quickly tends to be the Mott insulator with further increasing of x with $x \geq x_c$ within this narrow region, which shows that the three-body repulsive on-site interaction in this case resists against the system becoming the Mott insulator till the system almost reaches the Fock regime. Moreover, one can expect that the quantum phase crossover due to finite number of bosons in the system will be enhanced with further increasing of the number of bosons as shown in [22].

As shown in [10] for the phase diagram of the model, the local three-body interaction in the Bose–Hubbard model does not change the characteristic properties of the phase transition with only the superfluid and the Mott insulator phase as emerging in the standard Bose–Hubbard model, which is consistent to the results shown in the early work using the mean-field approximation [11] and the later work using the density matrix renormalization group method [12]. Specifically, the local three-body interaction

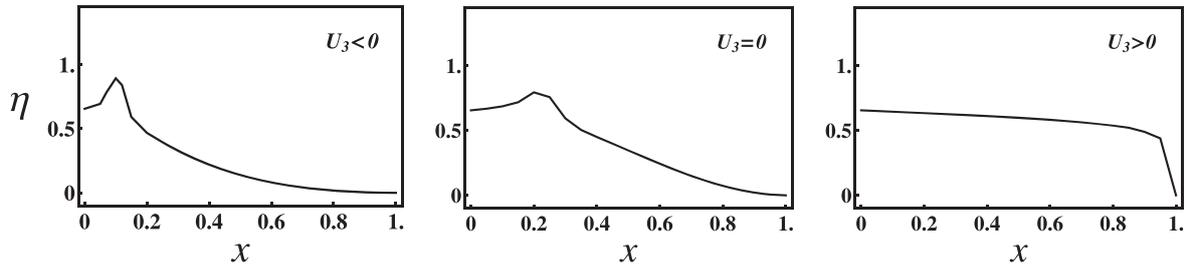


Figure 2. The ground-state entanglement measure of the two-site Bose–Hubbard model with attractive two-body on-site interaction and three-body on-site interaction with $U_3 < 0$, $U_3 = 0$, and $U_3 > 0$, respectively, as function of x for $N = 100$ bosons.

only alters the size and boundaries of the Mott robes and the position of the critical point [10–12], with which the result shown in this work is consistent. In addition, the situation will certainly become complicated when the three-body tunneling terms are considered, with which, besides the critical point shift, a phase-locking state appears even only up to two-body tunneling included as concluded in [30].

In order to further elucidate the system evolution with the variation of the control parameter x , the von Neumann entropy defined by

$$\eta = -\text{Tr}(\rho_1 \log_{N+1} \rho_1) = -\text{Tr}(\rho_2 \log_{N+1} \rho_2) \quad (11)$$

as the entanglement measure for the ground state of system is also calculated, where ρ_1 is the reduced density matrix obtained by taking the partial trace over the subsystem of a_2 -bosons, and similarly for ρ_2 . Here we use the logarithm to the base $N + 1$ instead of base 2 to ensure that the maximal measure is normalized to 1. Figure 2 shows the ground-state entanglement measure of the system as a function of x for $N = 100$ bosons. It is obvious that there is always a peak in the measure within the critical region when $U_3 \leq 0$, which is consistent with the so-called critical point entanglement [31]. Most noticeably, the peak of the measure becomes sharper, and the maximum value of the measure increases when $U_3 < 0$. It is expected that the entanglement measure at the critical point will approach to its maximal value with further increasing of $|U_3|$ for $U_3 < 0$. On the contrary, the entanglement measure gradually decreases with the increasing of x for $x \leq x_c$ with $x_c \sim 0.92$, while it drops down rapidly with the increasing of x when $x > x_c$. It is clear that the critical point entanglement disappears when the three-body on-site interaction is repulsive, and the maximum value of the measure, which is now far less than its maximal value, is at the Rabi regime with $x = 0$ in this case, of which the situation is quite similar to the case of the standard BHM with the repulsive two-body on-site interaction.

4. Summary

In summary, it is shown the extended one-dimensional dimer Bose–Hubbard model with multi-body interactions can be solved exactly by using the algebraic Bethe ansatz mainly

due to the site-permutation S_2 symmetry. The solution for the model with up to three-particle hopping and three-body on-site interaction is explicitly provided. Though the solution is demonstrated for the model with up to three-body interactions only, it is obvious that the one-dimensional dimer EBHM with finite order multi-body interactions, which is equivalent to the extended LMG model with finite order multi-body interactions after the $SU(2)$ realization, is also exactly solvable due to the site-permutation S_2 symmetry. Lower part of the excitation energy levels and the ground-state entanglement measure of the standard BH Hamiltonian with the attractive two-body interaction plus the three-body on-site interaction for 100 bosons with variation of the control parameter are calculated by using the exact solution. It is shown that the attractive three-body on-site interaction reinforces the critical point entanglement of the standard BH model with the attractive two-body on-site interaction. Similar extensions of the model with multi-body interactions to a family of fragmented multi-state cases shown in [32] should also be possible. Since the entanglement is the most important resource for quantum technology, the results of this work may be helpful for design of an optical lattice for ultracold atoms [33] or a tuneable superconducting quantum interference device [34] with maximal entanglement. For example, in a system of ultracold bosonic atoms, not only two-body interactions can be tuned [35–37], the effective on-site three-body interaction emerging through virtual transitions of particles from the lowest energy band to higher energy bands may be controlled by changing the orbital’s density profile [33]. Moreover, as shown in [34], the hopping interactions in a circuit QED device of two superconducting transmon qubits can also be tuned via a non-linear cross-Kerr interactions. It is expected that the local three-body interaction may also be tuneable in a nonlinear superconducting quantum interference device. On the other hand, when q -body interactions with $q_{\max} \geq 3$ are included in the standard BH model, the corresponding extended Heine–Stieltjes polynomials in determining the solution should satisfy a q_{\max} -th order differential equation [25], which, together with further numerical analysis of the model, will be studied in our future work.

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