

# Hierarchical algebraic structure and recursive solution of the Bose-Hubbard model

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We uncover a previously unrecognized hierarchical algebraic structure in the Bose-Hubbard model that enables a systematic construction of its spectrum without relying on integrability. We develop a recursive framework in which, within each fixed particle-number sector, the eigenproblem of a  $p$ -site system is reduced to a closed set of algebraic relations determined entirely by the eigenpairs and single-particle transfer amplitudes of the  $(p - 1)$ -site subsystem. This reduction yields two complementary sets of Bethe-type equations whose solutions exhaust the spectrum. The underlying structure originates from the locality of the Hamiltonian, which constrains the coupling between subsystems and gives rise to an emergent sparse, near-tridiagonal representation of the many-body problem. As an explicit demonstration, we construct the complete spectrum of the three-site Bose-Hubbard model from that of the two-site system for particle numbers  $n \leq 3$ , obtaining exact agreement with direct diagonalization. The resulting formulation substantially reduces computational cost and reveals a form of hierarchical solvability in a nonintegrable quantum many-body system. More broadly, our results suggest that recursive algebraic constructions may provide a general framework for analyzing lattice models beyond the conventional integrable paradigm.

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## I. INTRODUCTION

Understanding the structure and solvability of quantum many-body Hamiltonians remains a central challenge across condensed-matter physics, quantum optics, and statistical mechanics [1–5]. While exact solutions are available for a limited class of integrable models through techniques such as the Bethe ansatz and related algebraic methods [6–8], most physically relevant lattice systems are nonintegrable and therefore rely on numerical calculations or approximate analytical treatments. A fundamental question is whether nonintegrable many-body systems may nevertheless possess hidden algebraic structures that permit systematic and efficient construction of their spectra.

The Bose-Hubbard model (BHM) provides an ideal setting in which to explore this question. As the prototypical model of interacting bosons on a lattice [9,10], it captures the competition between kinetic delocalization and on-site interactions and serves as the standard theoretical description of ultracold bosonic atoms in optical lattices [3,11]. The model has played a central role in studies of quantum phase transitions, strongly correlated bosonic matter, and nonequilibrium

dynamics [12,13]. Owing to its representative structure, the BHM has also become a benchmark platform for a broad range of numerical many-body techniques, including quantum Monte Carlo simulations, density-matrix renormalization group methods, tensor-network approaches, and dynamical mean-field theories [14–18]. Despite its simple form, the generic BHM is nonintegrable [10,19]. The dimension of the Hilbert space grows rapidly with both particle number and lattice size, rendering exact diagonalization increasingly demanding. Consequently, most investigations rely on approximate approaches such as strong-coupling expansions [20], mean-field theories [21], semiclassical methods [22], or advanced numerical simulations. Exact analytical results remain comparatively scarce and are generally restricted to special limits, low-dimensional sectors, or systems possessing additional symmetries.

The search for exact solutions of the BHM has a long history. Early attempts were motivated by the success of the Lieb-Liniger model [23,24] and employed coordinate Bethe-ansatz techniques [25]. However, Choy and Haldane showed that the lattice BHM exhibits subtle complications associated with multiple site occupancy that prevent a straightforward coordinate Bethe-ansatz solution of the generic model [19]. The analysis in Ref. [19] reveals a fundamental difficulty in applying the coordinate-space Bethe ansatz to the BHM. The coordinate Bethe-ansatz construction, following the approach introduced for lattice systems by Lieb and Wu [26], represents the many-body wave function as a superposition of plane waves characterized by pseudomomenta, with amplitudes related through permutations of the particle coordinates. Such a construction is applicable when the matching conditions

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arising from particle encounters can be consistently described in terms of factorized two-body scattering processes. For bosons on a lattice, however, an additional complication arises because three or more particles can simultaneously occupy the same lattice site. These multiple-occupancy configurations impose additional constraints on the wave function through the Schrödinger equation. As shown explicitly in Ref. [19], for more than three bosons, these constraints cannot, in general, be satisfied within a straightforward extension of the Lieb-Wu coordinate Bethe ansatz. In particular, the amplitudes generated by the Lieb-Wu Bethe-ansatz construction possess a factorized structure determined by pairwise combinations of pseudomomenta, whereas the constraints associated with multiple occupancy require a more general dependence that cannot be accommodated within the same ansatz. Haldane further showed that this difficulty cannot be removed simply by introducing a Hermitian effective multiparticle interaction. Such a modification would require the relevant off-diagonal amplitudes in pseudomomentum space to depend only on appropriate total combinations of pseudomomenta, whereas the amplitudes generated by the Lieb-Wu-type construction retain a more restrictive factorized dependence on pairwise momentum combinations. Consequently, Lieb-Wu Bethe-ansatz wave functions do not, in general, provide a complete description of the correlations associated with multiple bosonic occupancy of a lattice site. More generally, this difficulty reflects a mismatch between the restricted structure imposed by a factorized two-body-scattering ansatz and the full set of correlations permitted in the bosonic Hilbert space. While the Lieb-Wu construction naturally incorporates correlations generated through successive two-body scattering processes, multiple site occupancy can generate additional correlations that are not captured within the same ansatz. Thus, unrestricted multiple occupancy prevents a straightforward coordinate Bethe-ansatz solution of the generic BHM. Nevertheless, Bethe-type wave functions can still provide useful and accurate descriptions in special regimes. In particular, Krauth demonstrated that the coordinate Bethe ansatz can be successfully applied when the probability of multiple site occupancy remains sufficiently small [27]. These developments therefore established both the usefulness and the fundamental limitations of coordinate-space Bethe-ansatz approaches to lattice boson systems.

More recently, exact algebraic solutions have been obtained for a number of special Bose-Hubbard systems. In particular, the two-site (dimer) model admits an exact solution through the algebraic Bethe ansatz (ABA) [28,29], which exploits a realization of the underlying algebra directly in the bosonic Fock space rather than in coordinate space. The relation between this construction and Gaudin-type integrable models has been extensively studied [30]. The relation of the ABA with the associated extended Heine-Stieltjes polynomials for the dimer BHM was studied in Ref. [31]. The ABA framework has subsequently been used to investigate quantum critical behavior, correlation functions, nonlinear tunneling processes, and extensions involving higher-order interaction terms [32–35]. More recently, exact ABA solutions have also been obtained for homogeneous three-site (trimer) Bose-Hubbard systems [36].

Nevertheless, these developments remain closely tied to integrability or special algebraic symmetries, and no general framework is known that systematically relates the spectra of Bose-Hubbard systems with different numbers of lattice sites. The present work addresses precisely this issue. We show that the Bose-Hubbard model possesses a previously unnoticed hierarchical algebraic structure under site extension. Specifically, within each fixed particle-number sector, the eigenproblem of a  $p$ -site system can be constructed recursively from that of the  $(p - 1)$ -site subsystem through a closed set of algebraic relations involving subsystem eigenpairs and single-particle transfer amplitudes. The resulting formulation yields two complementary sets of Bethe-type equations whose solutions exhaust the spectrum. Unlike conventional Bethe-ansatz methods, however, the construction does not rely on integrability, factorized scattering, or the existence of an extensive set of conserved quantities. Instead, it emerges from the local structure of the Hamiltonian and the manner in which an additional lattice site couples to a previously solved subsystem. This recursive formulation reveals a highly structured organization of the many-body Hilbert space. In the resulting basis, the Hamiltonian acquires an emergent sparse, near-tridiagonal form, in sharp contrast to the comparatively dense matrices obtained in the conventional Fock basis. Beyond providing a new perspective on the spectral organization of the Bose-Hubbard model, this structure also leads to significant computational advantages.

To demonstrate the method, we explicitly construct the complete spectrum of the trimer Bose-Hubbard model from the exact solution of the dimer subsystem. The results are shown to agree exactly with direct diagonalization. We further demonstrate that the recursive formulation enables efficient truncation schemes in appropriate parameter regimes while maintaining high accuracy for low-energy states. More broadly, the existence of a recursive site-extension structure establishes a form of hierarchical solvability in a nonintegrable quantum many-body system and suggests a possible framework for analyzing a wider class of locally coupled lattice models.

## II. RECURSIVE CONSTRUCTION OF EIGENPAIRS OF THE BHM

Specifically, we consider the (one-dimensional) BH Hamiltonian on  $p$  lattice sites,

$$\hat{H}_p = -t \sum_{i=1}^{p-1} (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) - t (a_1^\dagger a_p + a_p^\dagger a_1)(1 - \delta_{p2}) + U \sum_{i=1}^p (\hat{n}_i)^2. \quad (1)$$

Here, “one dimensional” refers to a lattice geometry in which the sites are arranged in a chain, or equivalently a ring under periodic boundary conditions, with hopping restricted to nearest neighbors; this convention is assumed throughout, and “one dimensional” is omitted for brevity. In Eq. (1),  $t > 0$  is the uniform nearest-neighbor hopping amplitude and  $U$  is the on-site interaction strength. The operators  $a_i$  ( $a_i^\dagger$ ) are bosonic annihilation (creation) operators satisfying the

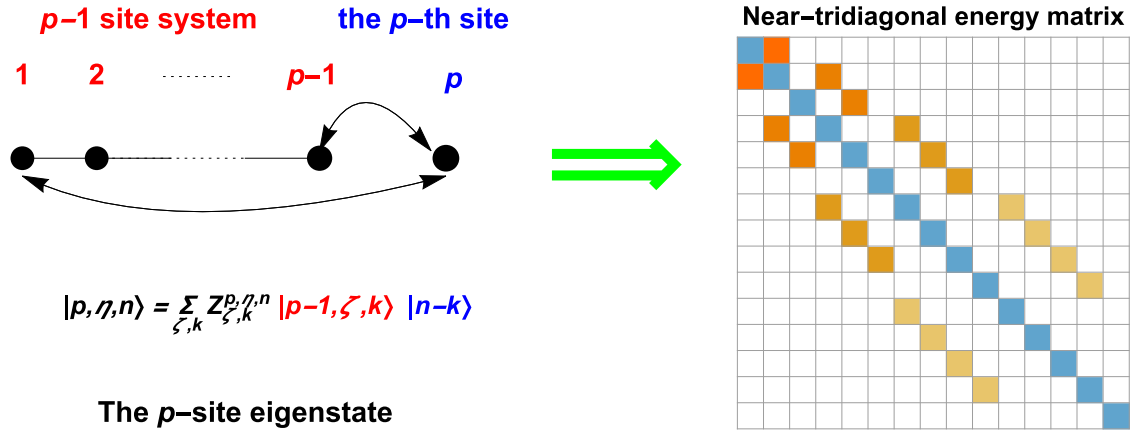


FIG. 1. Schematic illustration of the recursive construction of the  $p$ -site BHM from the  $(p-1)$ -site subsystem. Left: The  $p$ -site system is decomposed into a  $(p-1)$ -site subsystem coupled to the  $p$ th site. Particle hopping between the  $p$ th site and its neighboring sites (the first and the  $(p-1)$ th sites) is indicated by bidirectional arrows. In this representation, the eigenstates of the  $p$ -site system are expressed as linear combinations of tensor products of subsystem eigenstates and single-site Fock states. Right: On this basis, the Hamiltonian acquires an emergent sparse, near-tridiagonal structure, reflecting the constrained coupling between neighboring particle-number subsectors.

canonical commutation relations  $[a_i, a_j] = 0$  and  $[a_i, a_j^\dagger] = \delta_{ij}$ , while  $\hat{n}_i = a_i^\dagger a_i$  denotes the particle-number operator on site  $i$ . Periodic boundary conditions are imposed such that  $a_{p+m} = a_i$  for  $m = 0, 1, 2, \dots$  and  $i = 1, 2, \dots, p$ . The factor  $(1 - \delta_{p,2})$  avoids double counting of the hopping term in the two-site case.

It is straightforward to decompose the  $p$ -site Hamiltonian into a  $(p-1)$ -site subsystem coupled to the  $p$ th site,

$$\hat{H}_p = \hat{H}_{p-1} + U(\hat{n}_p)^2 - t a_p^\dagger (a_{p-1} + a_1(1 - \delta_{p,2})) - t(a_1^\dagger(1 - \delta_{p,2}) + a_{p-1}^\dagger)a_p, \quad (2)$$

where  $\hat{H}_{p-1}$  is the Hamiltonian of the  $(p-1)$ -site system with the same parameters  $t$  and  $U$  as demonstrated on the left in Fig. 1.

Since the total particle number  $\hat{n} = \sum_i \hat{n}_i$  is conserved, the spectrum can be classified by the particle number  $k$ . Assume that the eigenpairs of  $\hat{H}_{p-1}$  are known,  $\hat{H}_{p-1} |p-1, \zeta, k\rangle = E_{p-1, k}^{(\zeta)} |p-1, \zeta, k\rangle$ , for  $\zeta = 1, \dots, d_{p-1, k}$ , where the number of eigenstates corresponds to the Hilbert space dimension for  $k$  identical bosons on  $p-1$  sites,  $d_{p-1, k} = \frac{(k+p-2)!}{k!(p-2)!}$ . In the vacuum sector, one has  $E_{p-1, 0}^{(1)} = 0$ . The Hamiltonian (2) shows that site  $p$  couples to the remainder of the system exclusively through single-particle hopping operators. Consequently, an eigenstate of the  $p$ -site system with total particle number  $n$  can be expanded in the tensor-product basis formed by subsystem eigenstates and local Fock states:

$$|p, \eta, n\rangle = \sum_{k=0}^n \sum_{\zeta=1}^{d_{p-1, k}} Z_{\zeta, k}^{(p, \eta, n)} |p-1, \zeta, k; n-k\rangle, \quad (3)$$

as indicated at the bottom on the left of Fig. 1. Here,  $|p-1, \zeta, k; n-k\rangle = |p-1, \zeta, k\rangle |n-k\rangle$ , with  $|n-k\rangle = \frac{(a_p^\dagger)^{n-k}}{\sqrt{(n-k)!}} |0\rangle$  denoting the Fock state of  $n-k$  particles on the  $p$ th site. The index  $\eta = 1, \dots, d_{p, n}$  labels the eigenstates of

$\hat{H}_p$ , and the total number of expansion coefficients is

$$d_{p, n} = \sum_{k=0}^n d_{p-1, k} = \frac{(n+p-1)!}{n!(p-1)!}. \quad (4)$$

Substituting the expansion (3) into the eigenequation  $\hat{H}_p |p, \eta, n\rangle = E_{p, n}^{(\eta)} |p, \eta, n\rangle$  and projecting onto the basis states  $\langle p-1, \zeta, k; n-k|$  yields the coupled linear equations

$$\begin{aligned} & -t\sqrt{n-k} \sum_{\zeta'=1}^{d_{p-1, k+1}} \Lambda_{\zeta \zeta'}^{p-1, k} Z_{\zeta', k+1}^{(p, n, \eta)} \\ & -t\sqrt{n-k+1} \sum_{\zeta'=1}^{d_{p-1, k-1}} \Lambda_{\zeta' \zeta}^{p-1, k-1} Z_{\zeta', k-1}^{(p, n, \eta)} \\ & = Z_{\zeta, k}^{(p, n, \eta)} (E_{p, n}^{(\eta)} - U(n-k)^2 - E_{p-1, k}^{(\zeta)}), \end{aligned} \quad (5)$$

for  $k = 0, 1, \dots, n$  and  $\zeta = 1, 2, \dots, d_{p-1, k}$  for given  $k$ . Thus, once the  $(p-1)$ -site spectrum is known, the eigenproblem of the  $p$ -site Hamiltonian reduces to solving this closed system of linear equations. The key quantities appearing in Eq. (5) are the single-particle transfer amplitudes of the  $(p-1)$ -site subsystem,

$$\Lambda_{\zeta \zeta'}^{p-1, k} = \langle p-1, \zeta', k | (a_1(1 - \delta_{p,2}) + a_{p-1}) | p-1, \zeta, k+1 \rangle, \quad (6)$$

which can be calculated straightforwardly when the eigenstates of the  $(p-1)$ -site subsystem are completely known.

It follows from Eq. (5) that the eigenequations lead to a set of three-term recurrence relations among the expansion coefficients  $Z_{\zeta, k}^{(p, n, \eta)}$  with respect to the particle number  $k$  of the  $(p-1)$ -site subsystem. This structure closely resembles that of the dimer case [28,29]. As will be shown below, the resulting matrix, expressed in terms of the coefficients  $Z_{\zeta, k}^{(p, n, \eta)}$ , exhibits a predominantly tridiagonal band structure as indicated on the right of Fig. 1. This arises because only a limited number of coefficients with different  $\zeta$  are coupled, which likely underlies the computational efficiency of the recursive

scheme. In addition, Eq. (5) admits two distinct classes of solutions depending on whether the coefficient  $Z_{1,0}^{(p,n,\eta)}$  vanishes.

*Case I.*  $Z_{1,0}^{(p,n,\eta)} \neq 0$ . Without loss of generality, up to a normalization factor, we may set

$$Z_{1,0}^{(p,n,\eta)} = 1. \quad (7)$$

From Eq. (5) with  $k = 0$ , the eigenvalue is then obtained as

$$E_{p,n}^{(\eta)} = Un^2 - t\sqrt{n} \sum_{\zeta'=1}^{d_{p-1,1}} \Lambda_{1\zeta'}^{p-1,0} Z_{\zeta',1}^{(p,n,\eta)}. \quad (8)$$

The remaining expansion coefficients  $Z_{\zeta,k}^{(p,n,\eta)}$ , with  $k \neq 0$  must satisfy the coupled algebraic equations

$$\begin{aligned} & -t\sqrt{n-k} \sum_{\zeta'=1}^{d_{p-1,k+1}} \Lambda_{\zeta\zeta'}^{p-1,k} Z_{\zeta',k+1}^{(p,n,\eta)} - t\sqrt{n-k+1} \sum_{\zeta'=1}^{d_{p-1,k-1}} \Lambda_{\zeta'\zeta}^{p-1,k-1} Z_{\zeta',k-1}^{(p,n,\eta)} \\ & = Z_{\zeta,k}^{(p,n,\eta)} \left( U(2n-k)k - t\sqrt{n} \sum_{\zeta'=1}^{d_{p-1,1}} \Lambda_{1\zeta'}^{p-1,0} Z_{\zeta',1}^{(p,n,\eta)} - E_{p-1,k}^{(\zeta)} \right), \end{aligned} \quad (9)$$

for  $k = 1, 2, \dots, n$  and  $\zeta = 1, 2, \dots, d_{p-1,k}$ . We refer to Eqs. (8) and (9) as the type-I Bethe-type ansatz equations (BAEs). Solutions obtained from the type-I BAEs correspond exclusively to eigenpairs with  $Z_{1,0}^{(p,n,\eta)} \neq 0$ .

*Case II.*  $Z_{1,0}^{(p,n,\eta)} = 0$ . If  $Z_{1,0}^{(p,n,\eta)} = 0$ , Eq. (4) with  $k = 0$  imposes the constraint

$$\sum_{\zeta'=1}^{d_{p-1,1}} \Lambda_{1\zeta'}^{p-1,0} Z_{\zeta',1}^{(p,n,\eta)} = 0. \quad (10)$$

The  $Z_{\zeta,k}^{(p,n,\eta)}$  coefficients for  $k \geq 1$  and the eigenenergy  $E_{p,n}^{(\eta)}$  must also satisfy

$$-t\sqrt{n-k} \sum_{\zeta'=1}^{d_{p-1,k+1}} \Lambda_{\zeta\zeta'}^{p-1,k} Z_{\zeta',k+1}^{(p,n,\eta)} - t\sqrt{n-k+1} \sum_{\zeta'=1}^{d_{p-1,k-1}} \Lambda_{\zeta'\zeta}^{p-1,k-1} Z_{\zeta',k-1}^{(p,n,\eta)} = Z_{\zeta,k}^{(p,n,\eta)} (E_{p,n}^{(\eta)} - U(n-k)^2 - E_{p-1,k}^{(\zeta)}), \quad (11)$$

for  $k = 1, 2, \dots, n$  and  $\zeta = 1, 2, \dots, d_{p-1,k}$ . Equations (10) and (11) constitute the type-II BAEs.

The type-I and type-II BAEs are complementary: The former generate eigenpairs with  $Z_{1,0}^{(p,n,\eta)} \neq 0$ , while the latter describe those with  $Z_{1,0}^{(p,n,\eta)} = 0$ . Together they exhaust the full spectrum. Since Eqs. (8)–(11) are algebraically equivalent to the original eigenequations (5) of the  $p$ -site Hamiltonian; the total number of eigenpairs is exactly  $d_{p,n}$ . Therefore, the eigenproblem of the  $p$ -site Hamiltonian reduces to a closed algebraic system once the spectrum and transfer amplitudes of the  $(p-1)$ -site system are known. Consequently, the  $p$ -site BHM can be solved recursively through the type-I and type-II BAEs. Since the  $p = 1$  system is trivial, mathematical induction ensures that the BHM with an arbitrary number of sites  $p$  is exactly solvable.

### III. EXPLICIT CONSTRUCTION FOR DIMER AND TRIMER SYSTEMS

We now illustrate the recursive procedure by constructing the exact spectra of the dimer ( $p = 2$ ) and trimer ( $p = 3$ ) systems. The starting point is the trivial single-site case ( $p = 1$ ), with Hamiltonian  $\hat{H}_1 = U\hat{n}_1^2$ , eigenenergies  $E_{1,k}^{(1)} = Uk^2$ , and corresponding eigenstates  $|p = 1, k\rangle = (1/\sqrt{k!})(a_1^\dagger)^k|0\rangle$ , where the additional label  $\zeta = 1$  can be omitted.

#### A. The dimer system

For the two-site (dimer) system, the general formalism shown previously simplifies considerably. The transfer

amplitudes of the single-site subsystem are  $\Lambda^{1,k} = \sqrt{k+1}$ , and the subsystem eigenenergy  $E_{1,0}^{(1)} = 0$ . The dimer model admits only type-I solutions. If  $Z_0^{(2,n,\eta)} = 0$ , Eq. (10) forces  $Z_1^{(2,n,\eta)} = 0$ , and the recurrence (11) then yields vanishing coefficients for all  $k$ , corresponding only to the trivial null vector. Nontrivial solutions therefore require  $Z_0^{(2,n,\eta)} \neq 0$ , and we may set  $Z_0^{(2,n,\eta)} = 1$  up to a normalization constant. Thus, the eigenproblem reduces to the coupled equations:

$$\begin{aligned} & -t\sqrt{(k+1)(n-k)} Z_{k+1}^{(2,n,\eta)} - t\sqrt{k(n-k+1)} Z_{k-1}^{(2,n,\eta)} \\ & = Z_k^{(2,n,\eta)} (2U(n-k)k - t\sqrt{n} Z_1^{(2,n,\eta)}), \end{aligned} \quad (12)$$

for  $k = 1, 2, \dots, n$ , with the eigenenergy given by

$$E_{2,n}^{(\eta)} = Un^2 + t\sqrt{n} Z_1^{(2,n,\eta)}. \quad (13)$$

Equation (12) is a three-term recurrence that expresses  $Z_{k+1}^{(2,n,\eta)}$  for  $k = 1, \dots, n-1$  recursively as a polynomial in  $Z_1^{(2,n,\eta)}$  of degree  $k+1$ . The final relation for  $k = n$  then yields a polynomial equation of degree  $n+1$  in  $Z_1^{(2,n,\eta)}$ . Consequently, there are exactly  $n+1$  eigenenergies  $E_{2,n}^{(\eta)}$  for fixed particle number  $n$ , labeled by  $\eta = 1, 2, \dots, n+1$ .

Actually, the Bethe-ansatz states used in Refs. [28–30,32] and the eigenstate expansion adopted in Eq. (3) with  $p = 2$  provide two different parametrizations of the same Hilbert-space eigenvectors. For example, the Bethe-ansatz eigenstates

used in Refs. [30,32] for the dimer BHM are

$$|\eta; n\rangle = \prod_{i=1}^{(n-v_1-v_2)/2} S^\dagger(y_i^{(\eta)}) a^{\dagger v_1} b^{\dagger v_2} |0\rangle, \quad (14)$$

where  $v_1, v_2 = 0$  or  $1$  are chosen such that  $n - v_1 - v_2$  is even, and

$$S^\dagger(y) = \frac{1}{1+y} a^{\dagger 2} + \frac{1}{1-y} b^{\dagger 2}, \quad (15)$$

with

$$a^\dagger = \frac{1}{\sqrt{2}}(a_1^\dagger + a_2^\dagger), \quad b^\dagger = -\frac{i}{\sqrt{2}}(a_1^\dagger - a_2^\dagger). \quad (16)$$

Upon expanding Eq. (14) in the original bosonic operators  $a_1^\dagger$  and  $a_2^\dagger$ , one obtains a linear combination of the same Fock states appearing in Eq. (3), with  $p = 2$ . Hence, up to a unitary transformation, the expansion coefficients  $Z_k^{(2,n,\eta)}$  appearing in Eq. (3) can therefore be expressed in terms of the Bethe roots  $\{y_i^{(\eta)}\}$  appearing in Eq. (14), establishing a one-to-one correspondence between the two descriptions.

Consequently, although the recursive formulation and the algebraic Bethe-ansatz approach employ different variables

and derive different sets of algebraic equations, they ultimately encode the same finite eigenvalue problem. The matching complexity and root counting therefore reflect a common underlying Hilbert-space structure rather than a coincidence. In particular, both Eqs. (12) and (13) and the Bethe equations of Refs. [28–30,32] must generate exactly the same number of independent eigenstates in each particle-number sector. The agreement in the number of roots is thus a consequence of completeness of the two parametrizations of the same eigenspace. In fact, the algebraic Bethe-type construction for the dimer ( $p = 2$ ) system presented in this subsection can be extended to the BHM with an arbitrary number of sites,  $p \geq 3$ , as discussed in Appendix A.

### B. The trimer system

For  $p \geq 3$ , both type-I and type-II solutions appear, reflecting the richer algebraic structure of the system. For the trimer, the input required from the dimer subsystem consists of the eigenenergies  $E_{2,k}^{(\zeta)}$  for particle numbers  $k = 0, 1, \dots, n$  and  $\zeta = 1, 2, \dots, k+1$  for given  $k$ , and the single-particle transfer amplitudes  $\Lambda_{\zeta'\zeta}^{2,k}$  defined in Eq. (6), which for the dimer is given by

$$\begin{aligned} \Lambda_{\zeta'\zeta}^{2,k} &= \langle 2, \zeta', k | (a_1 + a_2) | 2, \zeta, k+1 \rangle \\ &= \sum_{m=0}^k (\tilde{Z}_m^{(2,k,\zeta')*} \tilde{Z}_{m+1}^{(2,k+1,\zeta)} \sqrt{m+1} + \tilde{Z}_m^{(2,k,\zeta')*} \tilde{Z}_m^{(2,k+1,\zeta)} \sqrt{k+1-m}). \end{aligned} \quad (17)$$

Here,  $\tilde{Z}_m^{(2,k,\zeta)}$  are the normalized expansion coefficients of the dimer eigenstates, with  $\tilde{Z}_m^{(2,0,\zeta)} = \delta_{m0} \delta_{\zeta 1}$  for the vacuum sector.

For type-I solutions, we set  $Z_{1,0}^{(3,n,\eta)} = 1$ . The eigenenergy is then given by

$$E_{3,n}^{(\eta)} = U n^2 - t \sqrt{n} \sum_{\zeta'=1}^2 \Lambda_{1\zeta'}^{2,0} Z_{\zeta'1}^{(3,n,\eta)}, \quad (18)$$

where the sum runs over the two dimer eigenstates in the one-particle sector ( $k = 1$ ). The remaining expansion coefficients  $Z_{\zeta,k}^{(3,n,\eta)}$  must satisfy the type-I BAEs:

$$\begin{aligned} &-t \sqrt{n-k} \sum_{\zeta'=1}^{k+2} \Lambda_{\zeta\zeta'}^{2,k} Z_{\zeta'k+1}^{(3,n,\eta)} - t \sqrt{n-k+1} \sum_{\zeta'=1}^k \Lambda_{\zeta'\zeta}^{2,k-1} Z_{\zeta'k-1}^{(3,n,\eta)} \\ &= Z_{\zeta k}^{(3,n,\eta)} \left( U(2n-k)k - t \sqrt{n} \sum_{\zeta'=1}^2 \Lambda_{1\zeta'}^{2,0} Z_{\zeta'1}^{(3,n,\eta)} - E_{2,k}^{(\zeta)} \right), \end{aligned} \quad (19)$$

for  $k = 1, 2, \dots, n$  and  $\zeta = 1, 2, \dots, k+1$  for given  $k$ .

Type-II solutions are characterized by  $Z_{1,0}^{(3,n,\eta)} = 0$ , which, through Eq. (4), with  $k = 0$  imposes the constraint

$$\sum_{\zeta'=1}^2 \Lambda_{1\zeta'}^{2,0} Z_{\zeta'1}^{(3,n,\eta)} = 0. \quad (20)$$

The coefficients  $\{Z_{\zeta k}^{(3,n,\eta)}\}$  for  $k \geq 1$  and the eigenenergy  $E_{3,n}^{(\eta)}$  should also satisfy

$$-t \sqrt{n-k} \sum_{\zeta'=1}^{k+2} \Lambda_{\zeta\zeta'}^{2,k} Z_{\zeta'k+1}^{(3,n,\eta)} - t \sqrt{n-k+1} \sum_{\zeta'=1}^k \Lambda_{\zeta'\zeta}^{2,k-1} Z_{\zeta'k-1}^{(3,n,\eta)} = Z_{\zeta k}^{(3,n,\eta)} (E_{3,n}^{(\eta)} - U(n-k)^2 - E_{2,k}^{(\zeta)}), \quad (21)$$

TABLE I. Eigenenergies  $\tilde{E}_{2,n}^{(\eta)} = E_{2,n}^{(\eta)}/t$  and the corresponding  $\{Z_k^{(2,n,\eta)}\}$  values of the dimer BHM, with  $U/t = -0.2$  for  $n \leq 5$  and  $k \geq 1$ .

| $n$ | $\tilde{E}_{2,n}^{(\eta)}$                                                 | $Z_k^{(2,n,\eta)}$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
|-----|----------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1   | -1.2<br>0.8                                                                | $Z_1^{(2,1,1)} = 1$<br>$Z_1^{(2,1,2)} = -1$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| 2   | -2.609 98<br>-0.8<br>1.409 98                                              | $Z_1^{(2,2,1)} = 1.279\ 846$ , $Z_2^{(2,2,1)} = 1$<br>$Z_1^{(2,2,2)} = 0$ , $Z_2^{(2,2,2)} = -1$<br>$Z_1^{(2,2,3)} = -1.562\ 688$ , $Z_2^{(2,2,3)} = 1$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| 3   | -4.233 03<br>-2.627 11<br>-0.566 97<br>1.827 11                            | $Z_1^{(2,3,1)} = 1.404\ 711$ , $Z_2^{(2,3,1)} = 1.404\ 711$ , $Z_3^{(2,3,1)} = 1$<br>$Z_1^{(2,3,2)} = 0.477\ 530$ , $Z_2^{(2,3,2)} = -0.477\ 530$ , $Z_3^{(2,3,2)} = -1$<br>$Z_1^{(2,3,3)} = -0.711\ 890$ , $Z_2^{(2,3,3)} = -0.711\ 890$ , $Z_3^{(2,3,3)} = 1$<br>$Z_1^{(2,3,4)} = -2.094\ 110$ , $Z_2^{(2,3,4)} = 2.094\ 110$ , $Z_3^{(2,3,4)} = -1$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| 4   | -6.073 98<br>-4.688 06<br>-2.775 82<br>-0.511 94<br>2.049 79               | $Z_1^{(2,4,1)} = 1.436\ 988$ , $Z_2^{(2,4,1)} = 1.573\ 494$ , $Z_3^{(2,4,1)} = 1.436\ 988$ , $Z_4^{(2,4,1)} = 1$<br>$Z_1^{(2,4,2)} = 0.744\ 031$ , $Z_2^{(2,4,2)} = 0$ , $Z_3^{(2,4,2)} = -0.744\ 031$ , $Z_4^{(2,4,2)} = -1$<br>$Z_1^{(2,4,3)} = -0.212\ 092$ , $Z_2^{(2,4,3)} = -0.883\ 672$ , $Z_3^{(2,4,3)} = -0.212\ 092$ , $Z_4^{(2,4,3)} = 1$<br>$Z_1^{(2,4,4)} = -1.344\ 031$ , $Z_2^{(2,4,4)} = 0$ , $Z_3^{(2,4,4)} = 1.344\ 031$ , $Z_4^{(2,4,4)} = -1$<br>$Z_1^{(2,4,5)} = -2.624\ 896$ , $Z_2^{(2,4,5)} = 3.523\ 300$ , $Z_3^{(2,4,5)} = -2.624\ 896$ , $Z_4^{(2,4,5)} = 1$                                                                                                                                                                                                                                                                                                                                   |
| 5   | -8.140 71<br>-6.992 12<br>-5.219 09<br>-3.084 86<br>-0.640 194<br>2.076 98 | $Z_1^{(2,5,1)} = 1.404\ 57$ , $Z_2^{(2,5,1)} = 1.563\ 625$ , $Z_3^{(2,5,1)} = 1.563\ 625$ , $Z_4^{(2,5,1)} = 1.404\ 57$ , $Z_5^{(2,5,1)} = 1$<br>$Z_1^{(2,5,2)} = 0.890\ 904$ , $Z_2^{(2,5,2)} = 0.340\ 884$ , $Z_3^{(2,5,2)} = -0.340\ 884$ , $Z_4^{(2,5,2)} = -0.890\ 904$ , $Z_5^{(2,5,2)} = -1$<br>$Z_1^{(2,5,3)} = 0.097\ 981$ , $Z_2^{(2,5,3)} = -0.727\ 554$ , $Z_3^{(2,5,3)} = -0.727\ 554$ , $Z_4^{(2,5,3)} = 0.097\ 981$ , $Z_5^{(2,5,3)} = 1$<br>$Z_1^{(2,5,4)} = -0.856\ 475$ , $Z_2^{(2,5,4)} = -0.695\ 143$ , $Z_3^{(2,5,4)} = 0.695\ 143$ , $Z_4^{(2,5,4)} = 0.856\ 475$ , $Z_5^{(2,5,4)} = -1$<br>$Z_1^{(2,5,5)} = -1.949\ 765$ , $Z_2^{(2,5,5)} = 1.111\ 892$ , $Z_3^{(2,5,5)} = 1.111\ 892$ , $Z_4^{(2,5,5)} = -1.949\ 765$ , $Z_5^{(2,5,5)} = 1$<br>$Z_1^{(2,5,6)} = -3.164\ 924$ , $Z_2^{(2,5,6)} = 5.338\ 008$ , $Z_3^{(2,5,6)} = -5.338\ 008$ , $Z_4^{(2,5,6)} = 3.164\ 924$ , $Z_5^{(2,5,6)} = -1$ |

for  $k = 1, 2, \dots, n$  and  $\zeta = 1, 2, \dots, k + 1$  for given  $k$ .

The recursive procedure is completely general and applies to the model with arbitrary site number  $p$  and arbitrary nonzero parameters  $U$  and  $t$ . As a concrete numerical illustration of the construction, we choose  $U/t = -0.2$  throughout most of the examples presented below. This choice is made solely for demonstration purposes and does not reflect any restriction of the method to the attractive-interaction regime.

Starting from the dimer system ( $p = 2$ ), we solve the type-I BAEs (11) and (12), with  $Z_0^{(2,n,\eta)} = 1$ . Table I presents the resulting eigenenergies  $\tilde{E}_{2,n}^{(\eta)} = E_{2,n}^{(\eta)}/t$  and the corresponding unnormalized expansion coefficients  $Z_k^{(2,n,\eta)}$ , for  $k \geq 1$  and particle numbers  $n \leq 5$ . It can be verified that these coefficients are orthogonal with respect to the eigenstate index  $\eta$ .

From the dimer solutions, we compute the single-particle transfer amplitudes  $\Lambda_{\zeta'\zeta}^{2,k}$  via Eq. (6). Table II lists these amplitudes for particle numbers of the dimer subsystem up to  $k = 3$ , which serve as essential input for the trimer construction. Using these dimer data, we apply the recursive construction,

specifically Eqs. (14) and (15) with  $Z_0^{(2,n,\eta)} = 1$  and Eqs. 16 and (17) with  $Z_0^{(2,n,\eta)} = 0$  to obtain the exact eigenpairs of the trimer system ( $p = 3$ ) with the same interaction strength  $U/t = -0.2$ . Table III displays the resulting eigenenergies  $\tilde{E}_{3,n}^{(\eta)} = E_{3,n}^{(\eta)}/t$  and the corresponding unnormalized expansion coefficients  $Z_{\zeta,k}^{(3,n,\eta)}$ .

Several observations from Tables II and III are noteworthy. First, as shown in Table II, only a few of the single-particle transfer amplitudes  $\{\Lambda_{\zeta'\zeta}^{2,k}\}$ , particularly those with  $\zeta = \zeta'$ , make significant contributions to the eigenequations (5). In general,  $\Lambda_{\zeta'\zeta}^{2,k}$  with  $|\zeta' - \zeta| \geq 4$  for  $k \geq 0$  are negligible, giving rise to the predominantly tridiagonal band structure of the matrix expressed in terms of the expansion coefficients  $Z_{\zeta,k}^{(p,n,\eta)}$ . Figure 2 presents bar plots of  $|\Lambda_{\zeta'\zeta}^{2,k}|$  as a function of  $\zeta$  for  $U/t = -0.2$ ,  $k = 10$ , and  $\zeta' = 2, 4, 5, 7$ , clearly showing that only a small number of amplitudes are non-negligible for each  $\zeta'$ . Second, the number of type-I solutions (with  $Z_{1,0}^{(3,n,\eta)} = 1$ ) consistently exceeds that of

TABLE II. The single-particle transfer amplitudes  $\{\Lambda_{\zeta'\zeta}^{2,k}\}$  of the dimer system with  $U/t = -0.2$  up to  $k = 3$ .

|                                                                                                                                                                  |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| $\Lambda_{11}^{2,0} = \sqrt{2}$ , $\Lambda_{12}^{2,0} = 0$                                                                                                       |
| $\Lambda_{11}^{2,1} = 1.997\ 52$ , $\Lambda_{12}^{2,1} = 0$ , $\Lambda_{13}^{2,1} = 0.099\ 6274$                                                                 |
| $\Lambda_{21}^{2,1} = 0$ , $\Lambda_{22}^{2,1} = \sqrt{2}$ , $\Lambda_{23}^{2,1} = 0$                                                                            |
| $\Lambda_{11}^{2,2} = -2.442\ 09$ , $\Lambda_{12}^{2,2} = 0$ , $\Lambda_{13}^{2,2} = 0.162\ 087$ , $\Lambda_{14}^{2,2} = 0$                                      |
| $\Lambda_{21}^{2,2} = 0$ , $\Lambda_{22}^{2,2} = 1.993\ 91$ , $\Lambda_{23}^{2,2} = 0$ , $\Lambda_{24}^{2,2} = -0.156\ 018$                                      |
| $\Lambda_{31}^{2,2} = 0.012\ 6028$ , $\Lambda_{32}^{2,2} = 0$ , $\Lambda_{33}^{2,2} = 1.417\ 66$ , $\Lambda_{34}^{2,2} = 0$                                      |
| $\Lambda_{11}^{2,3} = 2.812\ 32$ , $\Lambda_{12}^{2,3} = 0$ , $\Lambda_{13}^{2,3} = 0.234\ 084$ , $\Lambda_{14}^{2,3} = 0$ , $\Lambda_{15}^{2,3} = -0.001\ 869$  |
| $\Lambda_{21}^{2,3} = 0$ , $\Lambda_{22}^{2,3} = 2.432\ 16$ , $\Lambda_{23}^{2,3} = 0$ , $\Lambda_{24}^{2,3} = 0.245\ 462$ , $\Lambda_{25}^{2,3} = 0$            |
| $\Lambda_{31}^{2,3} = 0.031\ 811$ , $\Lambda_{32}^{2,3} = 0$ , $\Lambda_{33}^{2,3} = -1.998\ 46$ , $\Lambda_{34}^{2,3} = 0$ , $\Lambda_{35}^{2,3} = -0.202\ 971$ |
| $\Lambda_{41}^{2,3} = 0$ , $\Lambda_{42}^{2,3} = 0.015\ 680$ , $\Lambda_{43}^{2,3} = 0$ , $\Lambda_{44}^{2,3} = -1.422\ 71$ , $\Lambda_{45}^{2,3} = 0$           |

TABLE III. Eigenenergies  $\tilde{E}_{3,n}^{(\eta)} = E_{3,n}^{(\eta)}/t$  and the corresponding  $\{Z_{\zeta,k}^{(3,n,\eta)}\}$  values of the trimer BHM with  $U/t = -0.2$  for  $n \leq 3$ .

| $n$ | $\tilde{E}_{3,n}^{(\eta)}$ | $Z_{\zeta,k}^{(3,n,\eta)}$                                                                                                                                                                  |
|-----|----------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1   | -2.2                       | $Z_{1,0}^{(3,1,1)} = 1, Z_{1,1}^{(3,1,1)} = \sqrt{2}, Z_{2,1}^{(3,1,1)} = 0$                                                                                                                |
|     | 0.8                        | $Z_{1,0}^{(3,1,2)} = 1, Z_{1,1}^{(3,1,2)} = -1/\sqrt{2}, Z_{2,1}^{(3,1,2)} = 0$                                                                                                             |
|     | 0.8                        | $Z_{1,0}^{(3,1,3)} = 0, Z_{1,1}^{(3,1,3)} = 0, Z_{2,1}^{(3,1,3)} = 1$                                                                                                                       |
| 2   | -4.539 39                  | $Z_{1,0}^{(3,2,1)} = 1, Z_{1,1}^{(3,2,1)} = 1.869\ 69, Z_{2,1}^{(3,2,1)} = 0, Z_{1,2}^{(3,2,1)} = 1.935\ 69, Z_{2,2}^{(3,2,1)} = 0, Z_{3,2}^{(3,2,1)} = 0.031\ 3097$                        |
|     | -1.677 97                  | $Z_{1,0}^{(3,2,2)} = 1, Z_{1,1}^{(3,2,2)} = 0.438\ 988, Z_{2,1}^{(3,2,2)} = 0, Z_{1,2}^{(3,2,2)} = -0.940\ 86, Z_{2,2}^{(3,2,2)} = 0, Z_{3,2}^{(3,2,2)} = 0.014\ 1632$                      |
|     | -1.677 97                  | $Z_{1,0}^{(3,2,3)} = 0, Z_{1,1}^{(3,2,3)} = 0, Z_{2,1}^{(3,2,3)} = 0.620\ 821, Z_{1,2}^{(3,2,3)} = 0, Z_{2,2}^{(3,2,3)} = 1, Z_{3,2}^{(3,2,3)} = 0$                                         |
|     | 1.339 39                   | $Z_{1,0}^{(3,2,4)} = 1, Z_{1,1}^{(3,2,4)} = -1.069\ 69, Z_{2,1}^{(3,2,4)} = 0, Z_{1,2}^{(3,2,4)} = 0.541\ 032, Z_{2,2}^{(3,2,4)} = 0, Z_{3,2}^{(3,2,4)} = -1.509\ 71$                       |
|     | 1.477 97                   | $Z_{1,0}^{(3,2,5)} = 1, Z_{1,1}^{(3,2,5)} = -1.138\ 99, Z_{2,1}^{(3,2,5)} = 0, Z_{1,2}^{(3,2,5)} = 0.556\ 549, Z_{2,2}^{(3,2,5)} = 0, Z_{3,2}^{(3,2,5)} = 1.668\ 85$                        |
|     | 1.477 97                   | $Z_{1,0}^{(3,2,6)} = 0, Z_{1,1}^{(3,2,6)} = 0, Z_{2,1}^{(3,2,6)} = -1.610\ 770, Z_{1,2}^{(3,2,6)} = 0, Z_{2,2}^{(3,2,6)} = 1, Z_{3,2}^{(3,2,6)} = 0$                                        |
|     | -7.019 06                  | $Z_{1,0}^{(3,3,1)} = 1, Z_{1,1}^{(3,3,1)} = 2.130\ 674, Z_{2,1}^{(3,3,1)} = 0, Z_{1,2}^{(3,3,1)} = 2.916\ 153, Z_{2,2}^{(3,3,1)} = 0, Z_{3,2}^{(3,3,1)} = 0.046\ 964$                       |
| 3   | -4.304 07                  | $Z_{1,0}^{(3,3,1)} = -2.555\ 932, Z_{2,3}^{(3,3,1)} = 0, Z_{3,3}^{(3,3,1)} = 0.083\ 578, Z_{4,3}^{(3,3,1)} = 0$                                                                             |
|     | -4.304 07                  | $Z_{1,0}^{(3,3,2)} = 1, Z_{1,1}^{(3,3,2)} = 1.022\ 282, Z_{2,1}^{(3,3,2)} = -0.029\ 880, Z_{1,2}^{(3,3,2)} = -0.034\ 878, Z_{2,2}^{(3,3,2)} = -0.064\ 302, Z_{3,2}^{(3,3,2)} = 0.031\ 564$  |
|     | -4.304 07                  | $Z_{1,0}^{(3,3,3)} = 1.204\ 57, Z_{2,3}^{(3,3,3)} = -0.076\ 455, Z_{3,3}^{(3,3,3)} = 0.010\ 461, Z_{4,3}^{(3,3,3)} = 0.001\ 636$                                                            |
|     | -1.442 77                  | $Z_{1,0}^{(3,3,3)} = 1.204\ 57, Z_{2,3}^{(3,3,3)} = 24.5936, Z_{3,3}^{(3,3,3)} = 0.010\ 461, Z_{4,3}^{(3,3,3)} = -0.526\ 347$                                                               |
|     | -1.262 55                  | $Z_{1,0}^{(3,3,4)} = 1, Z_{1,1}^{(3,3,4)} = -0.145\ 838, Z_{2,1}^{(3,3,4)} = 0, Z_{1,2}^{(3,3,4)} = -0.804\ 820, Z_{2,2}^{(3,3,4)} = 0, Z_{3,2}^{(3,3,4)} = -0.671\ 955$                    |
|     | -1.262 55                  | $Z_{1,0}^{(3,3,4)} = -0.701\ 360, Z_{2,3}^{(3,3,4)} = 0, Z_{3,3}^{(3,3,4)} = -1.236\ 646, Z_{4,3}^{(3,3,4)} = 0$                                                                            |
|     | -1.262 55                  | $Z_{1,0}^{(3,3,5)} = 1, Z_{1,1}^{(3,3,5)} = -0.219\ 413, Z_{2,1}^{(3,3,5)} = -0.166\ 701, Z_{1,2}^{(3,3,5)} = -0.848\ 105, Z_{2,2}^{(3,3,5)} = -0.105\ 234, Z_{3,2}^{(3,3,5)} = 0.767\ 542$ |
|     | -1.262 55                  | $Z_{1,0}^{(3,3,5)} = -0.700\ 500, Z_{2,3}^{(3,3,5)} = 0.153\ 77, Z_{3,3}^{(3,3,5)} = 1.366\ 660, Z_{4,3}^{(3,3,5)} = 0.005\ 314$                                                            |
|     | 1.766 62                   | $Z_{1,0}^{(3,3,6)} = 1, Z_{1,1}^{(3,3,6)} = -0.219\ 413, Z_{2,1}^{(3,3,6)} = 12.568\ 500, Z_{1,2}^{(3,3,6)} = -0.848\ 104, Z_{2,2}^{(3,3,6)} = 7.934\ 150, Z_{3,2}^{(3,3,6)} = 0.767\ 524,$ |
|     | 1.766 62                   | $Z_{1,0}^{(3,3,6)} = -0.7005, Z_{2,3}^{(3,3,6)} = -11.593\ 500, Z_{3,3}^{(3,3,6)} = 1.366\ 660, Z_{4,3}^{(3,3,6)} = -0.400\ 651$                                                            |
|     | 1.766 62                   | $Z_{1,0}^{(3,3,7)} = 1, Z_{1,1}^{(3,3,7)} = -1.456\ 066, Z_{2,1}^{(3,3,7)} = -1.275\ 22, Z_{1,2}^{(3,3,7)} = 1.125\ 14, Z_{2,2}^{(3,3,7)} = 1.126\ 42, Z_{3,2}^{(3,3,7)} = -1.018\ 24$      |
|     | 1.766 62                   | $Z_{1,0}^{(3,3,7)} = 0.460\ 114, Z_{2,3}^{(3,3,7)} = -0.511\ 177, Z_{3,3}^{(3,3,7)} = 0.540\ 425, Z_{4,3}^{(3,3,7)} = -2.905\ 52$                                                           |
|     | 2.000 00                   | $Z_{1,0}^{(3,3,8)} = 1, Z_{1,1}^{(3,3,8)} = -1.456\ 066, Z_{2,1}^{(3,3,8)} = 0.651\ 626, Z_{1,2}^{(3,3,8)} = 1.125\ 14, Z_{2,2}^{(3,3,8)} = -0.575\ 588, Z_{3,2}^{(3,3,8)} = -1.018\ 24,$   |
|     | 2.000 00                   | $Z_{1,0}^{(3,3,8)} = 0.460\ 114, Z_{2,3}^{(3,3,8)} = 0.261\ 206, Z_{3,3}^{(3,3,8)} = 0.540\ 432, Z_{4,3}^{(3,3,8)} = 1.484\ 69$                                                             |
|     | 2.061 83                   | $Z_{1,0}^{(3,3,9)} = 0, Z_{1,1}^{(3,3,9)} = 0, Z_{2,1}^{(3,3,9)} = 1.108\ 15, Z_{1,2}^{(3,3,9)} = 0, Z_{2,2}^{(3,3,9)} = -1.108\ 15, Z_{3,2}^{(3,3,9)} = 0$                                 |
|     | 2.061 83                   | $Z_{1,0}^{(3,3,9)} = 0, Z_{2,3}^{(3,3,9)} = 0.477\ 525, Z_{3,3}^{(3,3,9)} = 0, Z_{4,3}^{(3,3,9)} = -1$                                                                                      |
|     | 2.061 83                   | $Z_{1,0}^{(3,3,10)} = 1, Z_{1,1}^{(3,3,10)} = -1.576\ 588, Z_{2,1}^{(3,3,10)} = 0, Z_{1,2}^{(3,3,10)} = 1.215\ 627, Z_{2,2}^{(3,3,10)} = 0, Z_{3,2}^{(3,3,10)} = 3.692\ 883$                |
|     | 2.061 83                   | $Z_{1,0}^{(3,3,10)} = 0.464\ 208, Z_{2,3}^{(3,3,10)} = 0, Z_{3,3}^{(3,3,10)} = -2.066\ 448, Z_{4,3}^{(3,3,10)} = 0$                                                                         |

type-II solutions (with  $Z_{1,0}^{(3,n,\eta)} = 0$ ), and this disparity grows with increasing particle number  $n$ . Importantly, the combined number of eigenpairs from type-I and type-II solutions exactly matches  $d_{3,n}$ , the dimension of the Hilbert subspace for  $n$  bosons on three sites, confirming the completeness of the construction. As an independent check, all results in Tables I and III were verified against direct numerical diagonalization in the original  $n$ -particle Fock basis [37], showing perfect agreement.

To demonstrate that the characteristic structure of the single-particle transfer amplitudes  $\Lambda_{\zeta'\zeta}^{2,k}$  is not limited to attractive interactions, Fig. 3 shows bar plots of  $|\Lambda_{\zeta'\zeta}^{2,k}|$  as functions of  $\zeta$  for  $U/t = 0.2$ ,  $k = 10$ , and  $\zeta' = 2, 4, 5, 7$ . Similar to the results displayed in Fig. 2 for  $U/t = -0.2$ , only a small subset of amplitudes remains appreciable for each  $\zeta'$ , while the majority are either vanishingly small or negligible. This indicates that the sparse coupling structure underlying the recursive formulation persists for both attractive and repulsive interactions.

It seems that the sparse near-tridiagonal structure emerging in the recursive formulation is a direct consequence of the locality and low rank of the single-particle transfer operator. For example, since the single-particle transfer operator  $a_1 + a_2$  modifies the subsystem by only one boson, it couples efficiently only a small subset of subsystem eigenstates with

similar internal structure. Consequently, most transfer amplitudes defined by Eq. (20) vanish identically or are strongly suppressed, leading to the observed sparse band structure of the recursive Hamiltonian.

To demonstrate the efficiency of the step-by-step recursive construction, we compare the CPU time required for the trimer with that of conventional brute-force matrix diagonalization in the original  $n$ -particle Fock basis. For the brute-force approach, the CPU time includes both the construction of the Hamiltonian matrix in the bosonic Fock basis  $\{|n_1, n_2, n_3\rangle\}$  with  $\sum_{i=1}^3 n_i = n$  and the subsequent matrix diagonalization. For the recursive construction, the CPU time includes the generation of the dimer eigenpairs and one-particle transfer amplitudes, as well as the solution of the trimer eigenequations (18)–(21). It should be emphasized that the CPU times reported here are obtained from Mathematica implementations of both the brute-force diagonalization and the recursive construction Supplemental Material [38]. To ensure a fair comparison, the same underlying algorithm is employed for generating the Hamiltonian matrix of the  $p$ -site BHM in both calculations, so that the observed performance difference originates primarily from the distinct representations of the eigenvalue problem rather than from differences in the matrix-construction procedure.

As stated previously, the computational cost of both the brute-force diagonalization and the recursive construction is

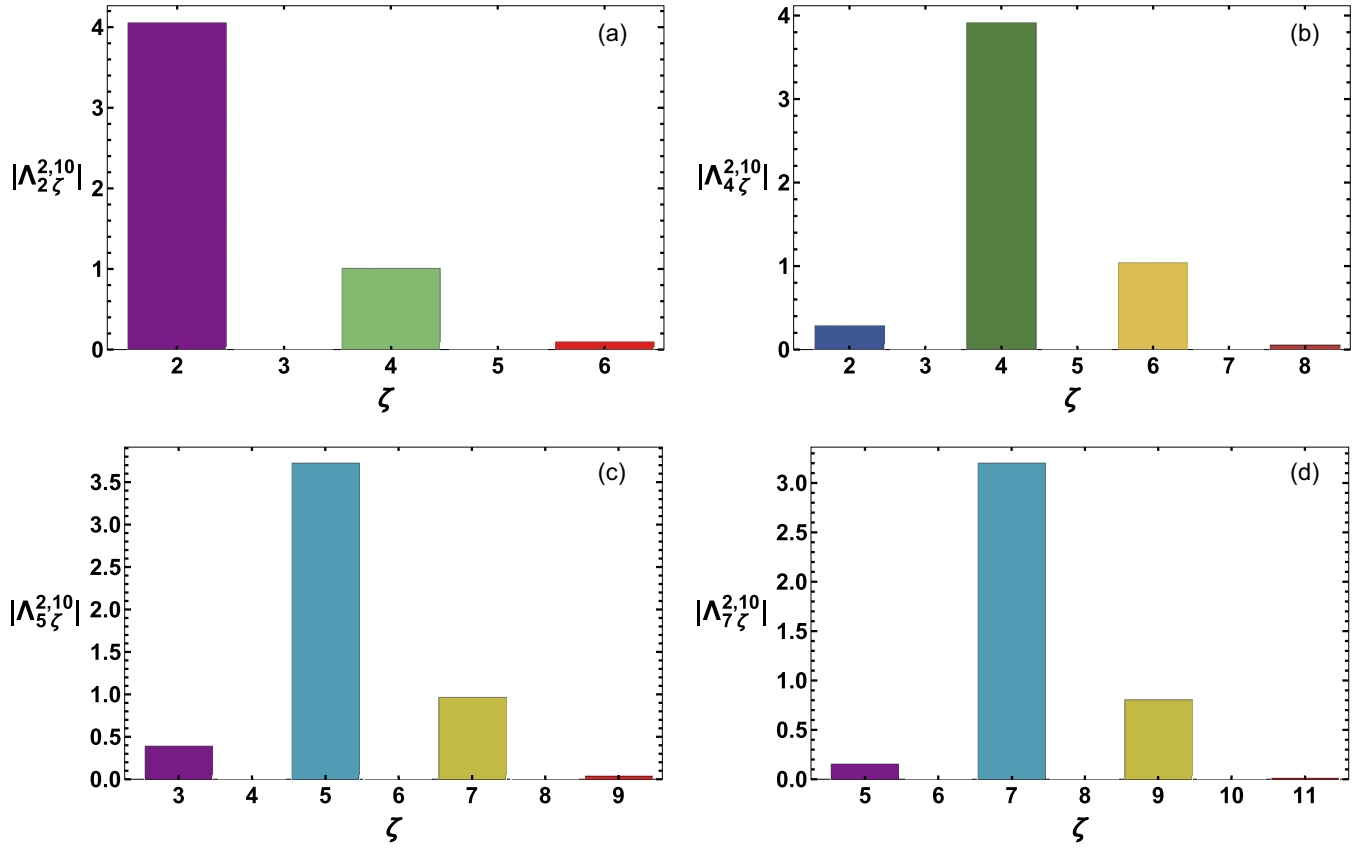


FIG. 2. Bar plots of  $|\Lambda_{\zeta\zeta'}^{2,k}|$  vs  $\zeta$  for  $U/t = -0.2$  and  $k = 10$ , with  $\zeta' = 2, 4, 5, 7$  shown in panels (a)–(d), respectively. Only amplitudes with significant contributions are displayed.

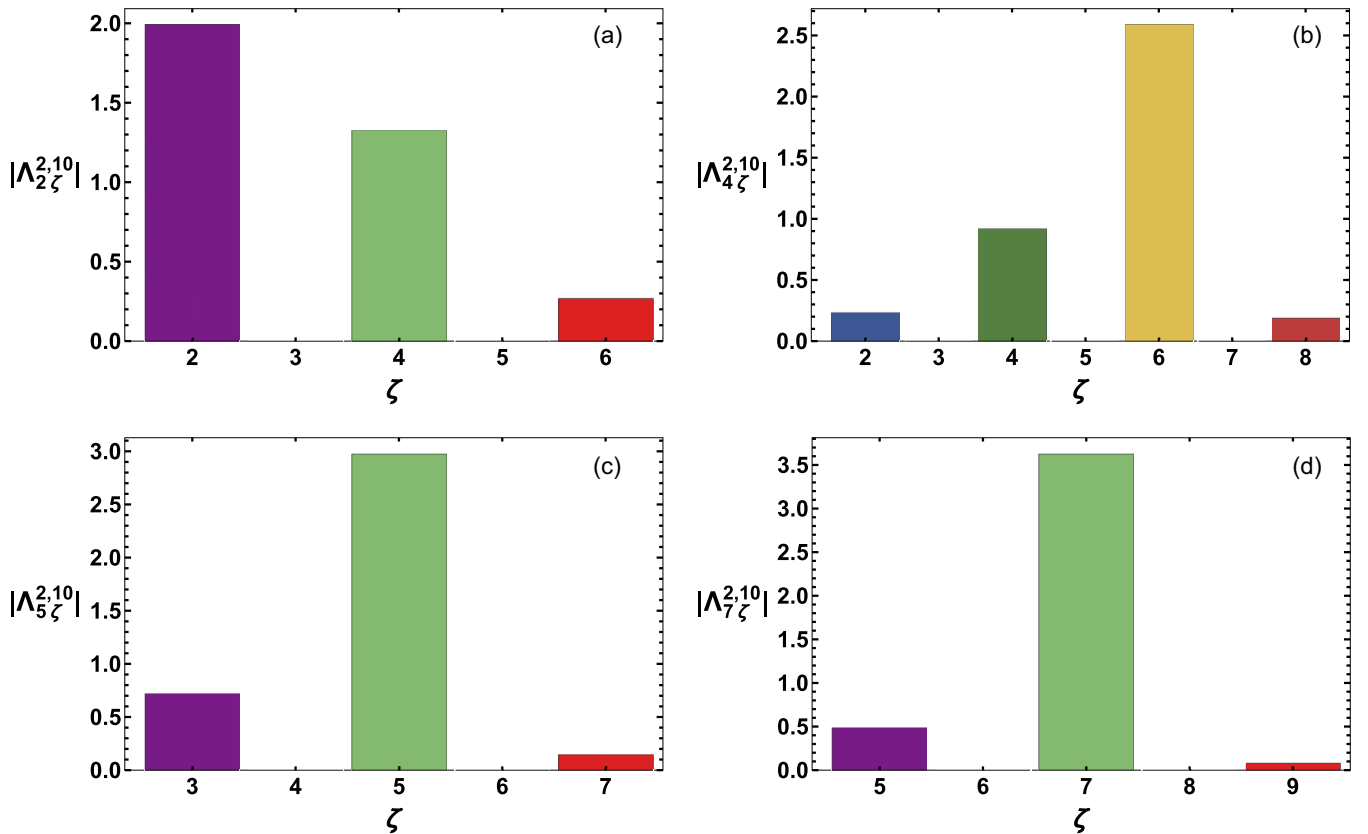


FIG. 3. The same as Fig. 2, but for  $U/t = 0.2$ .

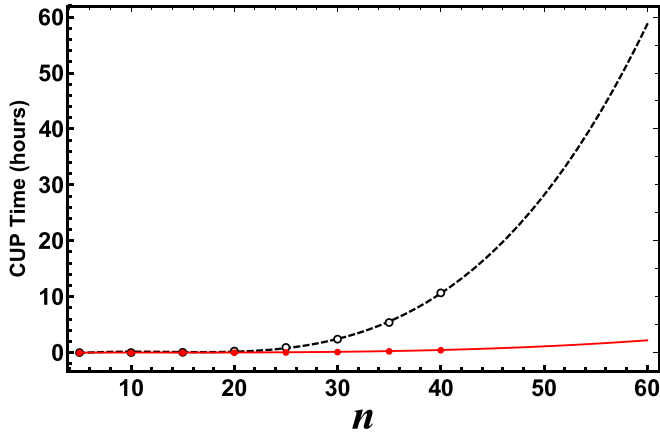


FIG. 4. CPU time vs particle number  $n$  for the recursive construction (red solid curve) and for conventional brute-force diagonalization in the original  $n$ -particle Fock basis (black dashed curve) for the trimer with  $U/t = -0.857\,14/n$ , illustrating the significant efficiency advantage of the recursive method.

largely insensitive to the specific finite nonzero value of  $U/t$ , apart from the trivial limits  $U = 0$  or  $t = 0$ . Figure 4 shows the CPU time required for the trimer with  $U/t = -0.857\,14/n$  as a function of  $n$ . The solid and open dots represent the recursive construction and brute-force diagonalization, respectively, while the corresponding curves are cubic polynomial fits to the data. All computations were performed in Mathematica on the same desktop PC (Intel Xeon E5-2687W v2, 128 GB RAM, Windows 10). It is evident that the recursive construction substantially reduces the computational cost as  $n$  increases. For example, at  $n = 40$ , the recursive scheme requires only 28.01 min, whereas brute-force diagonalization requires 10.67 h.

A similar behavior is observed for repulsive interactions ( $U > 0$ ). For example, for the trimer with  $U/t = 0.857\,14/n$  and  $n = 40$ , the recursive construction requires 29.44 min, which is very close to the 28.01 min obtained for the corresponding attractive case. Likewise, brute-force diagonalization requires 10.68 h for  $U/t = 0.857\,14/n$ , compared with 10.67 h for  $U/t = -0.857\,14/n$ . These results confirm that the computational efficiency of the recursive construction, as well as its advantage over brute-force diagonalization, is essentially independent of the sign and precise finite value of the interaction strength.

Although the Hamiltonian matrix has the same dimension in both methods for a given  $n$ , its structure differs significantly. In the recursive construction, the matrix expressed in terms of the expansion coefficients  $Z_{\zeta,k}^{(p,n,\eta)}$  from Eq. (5) is a sparse, predominantly tridiagonal band matrix. This arises from the three-term recurrence in particle number for fixed  $\zeta$  and the near vanishing of  $\Lambda_{\zeta'\zeta}^{2,k}$  for  $|\zeta' - \zeta| \geq 4$ . In contrast, the matrix constructed directly in the original Fock basis is comparatively dense. Consequently, diagonalization in the recursive framework is far more efficient, as the sparse, tridiagonal-dominating structure allows faster computation. In this approach, the Fock basis is effectively organized as a tensor product of the  $n$ -particle dimer eigenstates and single-site Fock states, and the CPU time required to compute the

single-particle transfer amplitudes from the known dimer eigenstates is negligible, explaining why the recursive construction outperforms brute-force diagonalization.

From a practical perspective, the dimension of the Hilbert space can be reduced further by exploiting permutation symmetry. Instead of working in the full Fock subspace with fixed total boson number  $n$ , the  $p$ -site BHM Hamiltonian may be decomposed into irreducible representations (irreps) of the permutation group  $S_p$ . The corresponding Hilbert space separates into symmetric, antisymmetric, and mixed-symmetry sectors, denoted by  $V_{p,S}$ ,  $V_{p,A}$ , and  $V_{p,M}$ , respectively. Since these symmetry-adapted subspaces have lower dimensions than the full  $n$ -boson space, diagonalization within a given irrep is generally more efficient.

For the dimer  $p = 2$ , the symmetric and antisymmetric sectors each have dimensions approximately equal to  $\text{Dim}(V_{2,n})/2$ , where  $\text{Dim}(V_{2,n}) = n + 1$  is the dimension of the full  $n$ -boson subspace. For the trimer  $p = 3$ , the dimension of the totally symmetric sector is  $\text{dim}(V_{3,S}) = \text{Round}[\frac{1}{12}n(n+6) + \frac{1}{8}(7 + (-1)^n) - \frac{\sqrt{12}}{9}|\sin(n/3)|]$ , where  $\text{Round}[x]$  denotes the nearest integer. In the large- $n$  limit,  $\text{Dim}(V_{3,S}) \sim n^2/12$ , and  $\text{Dim}(V_{3,M}) \sim n^2/3$ . Additional details are provided in Appendix A.

Accordingly, the trimer Hamiltonian may be treated either by direct diagonalization within the  $S_2$ -symmetric subspace [Eq. (B8)] or through the recursive construction formulated in the same symmetry-adapted basis [Eq. (B9)]. Mathematica implementations of both approaches are included in the Supplemental Material [38].

To assess their relative efficiency, we consider the trimer with  $n = 40$  bosons and  $U/t = -0.2$ . Using the code provided in the Supplemental Material [38], the complete set of dimer eigenpairs for  $0 \leq k \leq 40$  in the  $S_2$ -symmetric sector is obtained in 3.148 s. The evaluation of all single-particle transfer amplitudes  $\Lambda_{\zeta'\zeta}^{\text{Sym},k}$  according to Eqs. (B10)–(B12) requires 179.438 s. Combining these contributions with the CPU time needed for the final matrix diagonalization, the total CPU time required to obtain the trimer eigenpairs within the  $S_2$ -symmetric sector using the recursive construction [Eq. (B9)] is 200.727 s. In this estimate, the CPU time for the final matrix diagonalization in the  $S_2$ -symmetric subspace is conservatively taken to be the same as that required for diagonalization in the full bosonic Hilbert space for the trimer with  $n = 40$ . Because the  $S_2$ -symmetric sector has a smaller dimension, the actual diagonalization time is expected to be shorter. This is still substantially smaller than the 1680.55 s required by the recursive calculation performed in the full bosonic Hilbert space. By comparison, direct diagonalization within the same  $S_2$ -symmetric sector according to Eq. (B8) requires 882.078 s. These results demonstrate two important points. First, exploiting permutation symmetry significantly reduces the computational cost for both approaches by reducing the effective Hilbert-space dimension. Second, even after symmetry reduction, the recursive formulation remains more efficient than direct diagonalization, requiring approximately 4.4 times less CPU time in the present example. This indicates that the computational advantage of the recursive construction arises primarily from the sparse, near-tridiagonal structure that emerges naturally in the recursive

representation. This advantage persists both in the full Fock subspace and in the  $S_p$  symmetry-adapted subspaces, where the recursive formulation remains significantly more efficient than direct diagonalization.

The recursive construction is not limited to the trimer case. Once the eigenpairs and single-particle transfer amplitudes of the trimer system are obtained, the same procedure can be applied to construct the spectrum of the four-site ( $p = 4$ ) BHM with identical parameters. The formalism carries over directly: The  $p = 4$  eigenproblem reduces to solving the type-I and type-II Bethe-type equations, with the trimer eigenenergies  $E_{3,k}^{(\zeta)}$  and transfer amplitudes  $\Lambda_{\zeta'\zeta}^{3,k}$  as input. This stepwise construction can be iterated to systems with arbitrarily many sites, showing that the spectrum of the BHM can be systematically constructed through this recursive scheme. At present, however, a systematic comparison with symmetry-adapted exact diagonalization for  $p \geq 4$  has not been performed. Since the recursive approach reorganizes rather than reduces the Hilbert-space dimension, its ultimate computational scaling for larger systems remains to be established. Nevertheless, the emergent sparse structure of the recursive Hamiltonian and the reusability of subsystem data suggest promising opportunities for efficient implementations, particularly in conjunction with parallel computation.

### C. The ground state of the negative- $U$ trimer

In addition, owing to the predominantly tridiagonal structure of the matrix arising from the recursive construction, we find that the trimer Hamiltonian can be efficiently truncated when  $U < 0$ . We set the model parameters as  $t = (1 - x)t_0$  and  $U = -2xt_0/n$ , with  $x \in [0, 1]$ . As shown in Ref. [39], the negative- $U$  trimer exhibits a delocalized-to-clustered crossover at a critical point  $x_c \sim 0.5$  when  $n$  is finite. In this crossover regime, only a few low- $\zeta$  sectors of the matrix, expressed in terms of  $Z_{\zeta,k}^{(3,n,\eta)}$  in Eq. (5), are required for an accurate diagonalization. Our calculations indicate that truncation to the lowest  $\zeta$  sectors provides an excellent approximation, largely independent of the particle number  $n$ . Table IV compares the approximate and exact ground-state energies, as well as the absolute overlap  $\chi$  between the approximate and exact ground states, for the negative- $U$  trimer with  $n = 40$  at several values of  $x$ . The results show that contributions from large  $\zeta$  can be neglected in the ground state.

In particular, retaining only the  $\zeta = 1$  sector already yields a good approximation when  $x$  is far from the critical point  $x_c \sim 0.5$ . As  $x$  approaches  $x_c$ , additional  $\zeta$  sectors become relevant. For example, five- $\zeta$  sectors are required to achieve an absolute overlap  $\chi \geq 99.50\%$  at  $x = 0.5$ , indicating increased complexity of the ground state near criticality. While higher excited states are not well captured under such truncation, the ground state and its energy are reproduced with high accuracy.

In contrast, for  $U > 0$ , all  $\zeta$  sectors contribute significantly to the ground state across the entire parameter range, rendering truncation ineffective. Nevertheless, as shown in Table V, the CPU time required with and without truncation remains nearly the same for all  $x$ , due to the tridiagonal-dominant structure of the matrix generated by the recursive construction.

TABLE IV. Ground-state energy  $E_{3,n}^{(g)}/t_0$  of the negative- $U$  trimer with  $n = 40$ , obtained from the truncated calculation (Approx.) and exact calculation (Exact), together with the absolute ground-state overlap  $\chi$  with respect to the exact result, where  $t = (1 - x)t_0$  and  $U = -2xt_0/n$ . The number in parentheses indicates the number of lowest  $\zeta$  sectors retained to achieve  $\chi > 99.50\%$ .

| $x$ | Approx.      | Exact    | $\chi$   |
|-----|--------------|----------|----------|
| 0   | -80.0000 (1) | -80.0000 | 100%     |
| 0.1 | -74.8024 (1) | -74.8029 | 99.9952% |
| 0.2 | -69.6128 (1) | -69.6157 | 99.9652% |
| 0.3 | -64.4330 (1) | -64.4456 | 99.8126% |
| 0.4 | -59.2258 (3) | -59.3126 | 99.9669% |
| 0.5 | -54.3213 (5) | -54.3355 | 99.6673% |
| 0.6 | -54.5420 (1) | -54.5503 | 99.9117% |
| 0.7 | -58.9476 (1) | -58.9505 | 99.9744% |
| 0.8 | -65.0937 (1) | -65.0947 | 99.9920% |
| 0.9 | -72.2351 (1) | -72.2353 | 99.9986% |
| 1.0 | -80.0000 (1) | -80.0000 | 100%     |

## IV. CONCLUSION

We have developed a recursive construction that generates the eigenpairs of the  $p$ -site BH Hamiltonian from those of the  $(p - 1)$ -site subsystem through the associated single-particle transfer amplitudes. Within each fixed particle-number sector, the  $p$ -site eigenvalue problem reduces to two complementary sets of closed algebraic equations of Bethe type, whose solutions exhaust the full spectrum. As an explicit demonstration, we constructed the complete trimer spectrum from the dimer results for particle numbers  $n \leq 3$ , obtaining full agreement with direct diagonalization in the original Fock basis and thereby validating both the correctness and completeness of the approach.

A central feature of the construction is that only a restricted subset of the transfer amplitudes  $\{\Lambda_{\zeta'\zeta}^{p-1,k}\}$ , notably those with  $\zeta = \zeta'$ , contributes significantly to the  $p$ -site eigenproblem. This leads to an emergent sparse, predominantly tridiagonal band structure in the matrix representation with respect to the expansion coefficients. In contrast to the relatively dense matrices arising in the conventional Fock basis, this structure underlies a substantial reduction in computational cost and provides a clear explanation for the efficiency of the recursive scheme.

This tridiagonal-dominant structure also enables controlled truncation in the attractive ( $U < 0$ ) regime. For the trimer, we find that only a few low- $\zeta$  sectors are sufficient to accu-

TABLE V. CPU time (in seconds) required to compute the ground-state eigenpairs of the negative- $U$  trimer with  $U/t = -0.857\,14/n$  (corresponding to  $x = 0.3$ ) using the recursive construction, for particle numbers up to  $n = 40$ .

| $n$ | Approx.  | Exact    | $n$ | Approx. | Exact     |
|-----|----------|----------|-----|---------|-----------|
| 5   | 0.0938   | 0.1094   | 10  | 1.4219  | 1.4375    |
| 15  | 13.8906  | 14.1094  | 20  | 67.4688 | 68.2188   |
| 25  | 202.8280 | 204.8910 | 30  | 472.906 | 477.6090  |
| 35  | 938.8280 | 948.4840 | 40  | 1662.48 | 1680.5524 |

rately reproduce the ground-state eigenpair, with the required number increasing as the system approaches the critical point, reflecting enhanced correlations and the growing complexity of the ground state. In contrast, for repulsive interactions ( $U > 0$ ), all  $\zeta$  sectors contribute significantly to the ground state across the parameter range, rendering truncation ineffective. Nevertheless, the overall computational cost remains low due to the intrinsic sparsity of the recursive formulation.

More generally, the recursive construction reveals a hierarchical algebraic organization of the Bose-Hubbard model under site extension. Once the eigenpairs of the  $(p-1)$ -site subsystem are known, the  $p$ -site problem reduces to a finite set of algebraic relations determined entirely by lower-site data. This framework does not rely on integrability, yet provides a systematic route to constructing the spectrum iteratively. By mathematical induction, it applies to arbitrary system size, establishing a form of hierarchical solvability for the Bose-Hubbard model that extends beyond the conventional integrable paradigm [6–8]. It should be emphasized that the primary objective of the present work is to establish the recursive algebraic construction and to demonstrate its computational advantages for the systems studied here, rather than to provide a complete complexity analysis for arbitrarily large systems. Although the formalism can, in principle, be iterated to an arbitrary number of sites  $p$ , the numerical benchmarks presented in this work are restricted to the trimer. Consequently, the actual computational scaling of the recursive approach for  $p \geq 4$  has not yet been systematically established and remains an important subject for future investigation.

Nevertheless, several structural features of the construction suggest possible advantages as the system size increases. At each recursive step, the  $p$ -site problem is formulated entirely in terms of eigenpairs and single-particle transfer amplitudes of the  $(p-1)$ -site subsystem. These subsystem quantities can be generated once and subsequently reused in the construction of larger systems and in different calculations based on the same subsystem data. Moreover, the locality of the site-extension coupling gives rise to the sparse, near-tridiagonal structure of the recursive representation discussed above. Whether this structure remains sufficiently sparse to provide a substantial computational advantage for large  $p$  is a quantitative question that requires explicit investigation, but it provides a clear structural motivation for developing optimized implementations of the recursive method.

Some general observations concerning the size of the underlying Hilbert spaces can also be made. For a fixed particle number  $n$ , the dimension of the  $p$ -site bosonic Hilbert space,  $\mathcal{N}_{p,n}$  grows polynomially with  $p$  as  $\mathcal{N}_{p,n} \sim p^n/n!$  for large  $p$ . Conversely, for fixed  $p$ , it grows as  $n^{p-1}/(p-1)!$  for large  $n$ . When both  $p$  and  $n$  increase, the growth is combinatorial. These observations indicate that the potential computational advantage of the recursive formulation must ultimately be assessed relative to the particular scaling regime and to optimized symmetry-reduced or sparse-matrix implementations of conventional exact diagonalization.

The recursive construction also provides several opportunities for parallel computation. In particular, subsystem eigenproblems in different particle-number sectors, as well

as the associated single-particle transfer amplitudes, can be calculated independently and subsequently assembled at the next site-extension step. Once generated, these quantities can be stored and reused. The algebraic construction also separates naturally into the complementary type-I and type-II branches. These features suggest that an efficient parallel implementation may substantially improve the practical performance of the method, as has been demonstrated for related subsystem-based constructions in nuclear many-body calculations [40]. Developing such an implementation, together with a systematic comparison against optimized sparse and symmetry-adapted diagonalization methods for  $p \geq 4$ , constitutes an important direction for future work.

Finally, the underlying idea is not restricted to the BHM. More generally, many quantum many-body Hamiltonians are constructed from local degrees of freedom coupled through operators acting on neighboring subsystems. Examples include quantum spin chains [6–8] and fermionic or bosonic pairing models [41,42]. Whenever the coupling between an enlarged system and a previously solved subsystem can be expressed through a limited set of transition matrix elements, an analogous recursive organization of the eigenvalue problem may become possible. The present results therefore suggest a broader strategy for identifying hierarchical algebraic structures in quantum many-body systems and for exploiting locality, sparsity, and parallel computation to alleviate the computational challenges associated with conventional many-body approaches.

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## DATA AVAILABILITY

The Mathematica packages for generating the data used in this article are provided as Supplemental Material [38].

## APPENDIX A: ALGEBRAIC SOLUTION OF THE $p$ -SITE BHM

This Appendix establishes the general algebraic basis underlying the type-I and type-II equations introduced in Sec. III and clarifies why the corresponding construction is not restricted to the dimer. The argument applies to an arbitrary finite-dimensional eigenvalue problem and, consequently, to the BHM with an arbitrary number of sites and bosons.

Let  $\hat{A}$  be an  $\mathcal{N} \times \mathcal{N}$  complex matrix with matrix elements  $A_{ij}$ , and let  $\phi = (\phi_1, \phi_2, \dots, \phi_{\mathcal{N}})^T$  be an eigenvector associated with the eigenvalue  $E$ . The eigenvalue equation is

$$\hat{A}\phi = E\phi. \quad (\text{A1})$$

The construction below amounts to representing the eigenvector in different coordinate patches according to whether a selected component vanishes or not. Up to a permutation of the basis states, we distinguish two complementary cases.

*Case I.*  $\phi_1 \neq 0$ . In this case, the overall normalization of the eigenvector may be chosen such that  $\phi_1 = 1$ . The first

component of Eq. (A1) then gives

$$E = A_{11} + \sum_{l=1}^{\mathcal{N}-1} A_{1,l+1} \phi_{l+1}. \quad (\text{A2})$$

Substituting Eq. (A2) into the remaining  $\mathcal{N} - 1$  components of Eq. (A1) yields

$$A_{l+1,1} + \sum_{l'=1}^{\mathcal{N}-1} A_{l+1,l'+1} \phi_{l'+1} \times \left( A_{11} + \sum_{l'=1}^{\mathcal{N}-1} A_{1,l'+1} \phi_{l'+1} \right) \phi_{l+1} = 0, \quad (\text{A3})$$

for  $l = 1, 2, \dots, \mathcal{N} - 1$ . Equations (A2) and (A3) constitute a closed set of algebraic equations for the  $\mathcal{N} - 1$  independent components  $\phi_2, \dots, \phi_{\mathcal{N}}$  and the eigenvalue  $E$ . This defines the type-I solutions discussed in Sec. III.

*Case II.*  $\phi_1 = 0$ . The type-I construction does not include eigenvectors whose first component vanishes. To obtain this complementary set of solutions, we impose  $\phi_1 = 0$ . The first component of Eq. (A1) then gives the constraint

$$\sum_{l=1}^{\mathcal{N}-1} A_{1,l+1} \phi_{l+1} = 0, \quad (\text{A4})$$

whereas the remaining components satisfy

$$\sum_{l'=1}^{\mathcal{N}-1} A_{l+1,l'+1} \phi_{l'+1} - E \phi_{l+1} = 0, \quad l = 1, 2, \dots, \mathcal{N} - 1. \quad (\text{A5})$$

Equations (A4) and (A5) provide the complementary type-II solutions discussed in Sec. III.

The type-I and type-II constructions therefore cover the two possibilities  $\phi_1 \neq 0$  and  $\phi_1 = 0$  and, taken together, recover the complete spectrum of  $\hat{A}$ . If a different component is selected as the reference component, the same construction follows after a permutation of the basis. Thus, the algebraic formulation is not tied to any particular basis state or to any special property of the matrix  $\hat{A}$ .

The resulting equations have a structure analogous to Bethe-type equations in the sense that the spectral problem is transformed from a linear eigenvalue equation into a coupled set of nonlinear algebraic equations for a set of spectral variables, here represented by the component ratios of the eigenvector. Unlike the conventional Bethe ansatz, however, this construction does not assume integrability, factorized scattering, or an underlying Yang-Baxter structure. It is instead an exact algebraic reformulation of a finite-dimensional eigenvalue problem.

We now apply this general construction to the  $p$ -site BHM with a fixed total number  $n$  of bosons. In the occupation-number basis

$$|n_1, n_2, \dots, n_p\rangle, \quad \sum_{i=1}^p n_i = n, \quad (\text{A6})$$

the Hamiltonian is represented by an  $\mathcal{N}_{p,n} \times \mathcal{N}_{p,n}$  matrix, where

$$\mathcal{N}_{p,n} = \frac{(p+n-1)!}{n!(p-1)!}. \quad (\text{A7})$$

This is the dimension of the fixed- $n$  bosonic Hilbert space, which corresponds to the completely symmetric irreducible representation  $[n]$  of  $U(p)$ .

For the BHM Hamiltonian, the matrix elements  $H_{l'l}$ , where  $l$  and  $l'$  denote the occupation configurations  $n_1, \dots, n_p$  and  $n'_1, \dots, n'_p$ , respectively, are

$$\begin{aligned} H_{l'l} = & -t \sum_{i=1}^{p-1} \left[ \sqrt{(n_{i+1}+1)n_i} \delta_{n'_i, n_i-1} \delta_{n'_{i+1}, n_{i+1}+1} \right. \\ & + \sqrt{(n_i+1)n_{i+1}} \delta_{n'_{i+1}, n_{i+1}-1} \delta_{n'_i, n_i+1} \left. \right] \prod_{m \neq i, i+1}^p \delta_{n'_m, n_m} \\ & - t(1 - \delta_{p2}) \left[ \sqrt{(n_1+1)n_p} \delta_{n'_p, n_p-1} \delta_{n'_1, n_1+1} \right. \\ & + \sqrt{(n_p+1)n_1} \delta_{n'_1, n_1-1} \delta_{n'_p, n_p+1} \left. \right] \\ & \times \prod_{m \neq 1, p}^p \delta_{n'_m, n_m} + U \sum_{i=1}^p n_i^2 \prod_{l=1}^p \delta_{n'_l, n_l}. \end{aligned} \quad (\text{A8})$$

Upon identifying  $A_{l'l} = H_{l'l}$ , the general algebraic construction in Eqs. (A2)–(A5) provide an exact solution of the  $p$ -site BHM in every fixed- $n$  sector. In particular, the same two complementary sets of algebraic equations apply for arbitrary  $p$ ; increasing the number of sites changes only the dimension  $\mathcal{N}_{p,n}$  and the corresponding matrix elements, not the underlying algebraic construction.

This observation also clarifies the relation between the present formulation and the Bethe-ansatz descriptions discussed in the main text. For the dimer, the Bethe-ansatz vectors can be expanded in the same Fock-state basis used here, establishing a one-to-one correspondence between the Bethe roots and the expansion coefficients of the eigenvectors. The general algebraic construction above shows that the component-based formulation itself extends immediately to arbitrary  $p$ . The solution obtained in this manner is mathematically equivalent to direct diagonalization of  $\hat{H}$  in the  $\mathcal{N}_{p,n}$ -dimensional Fock subspace. Consequently, the combined type-I and type-II equations exhaust the complete spectrum.

It should be emphasized, however, that this general algebraic reformulation does not by itself eliminate the exponential growth of the many-body Hilbert space with increasing system size and particle number. As indicated by Eq. (A7), the number of algebraic variables increases rapidly with both  $p$  and  $n$ . The significance of the recursive construction developed in Sec. III is therefore not merely that it rewrites the eigenvalue problem algebraically, but that it reorganizes the problem through site extension in terms of lower-site eigenpairs and single-particle transfer amplitudes. The resulting recursive representation can exhibit the sparse, near-tridiagonal structure discussed in the main text, which

provides the basis for the computational advantages observed in the present calculations.

## APPENDIX B: EXACT DIAGONALIZATION OF THE DIMER AND TRIMER BHMS IN PERMUTATION-SYMMETRY-ADAPTED BASES

It is well known [35,36,39] that, instead of working in the full Fock space with fixed total boson number  $n$ , the  $p$ -site BHM Hamiltonian may be diagonalized within subspaces transforming according to the irreps of the permutation group  $S_p$ . The corresponding Hilbert space decomposes into symmetric, antisymmetric, and mixed-symmetry sectors, denoted by  $V_{p,S}$ ,  $V_{p,A}$ , and  $V_{p,M}$ , respectively. Since these symmetry-adapted subspaces generally have much smaller dimensions than the full  $n$ -boson Hilbert subspace, their use

can substantially reduce the computational cost. In this Appendix, we focus on the  $S_2$ -symmetric sectors of the dimer and trimer BHMs, which are used in the CPU-time comparisons discussed in the main text.

For the dimer BHM, the basis states spanning the symmetric subspace  $V_{2,S}$ , corresponding to the  $[2, 0]$  irrep of  $S_2$ , are generated by  $\{B_{2,1}^{\dagger n-2\mu} B_{2,2}^{\dagger \mu} |0\rangle\}$ , where  $B_{2,1}^{\dagger} = a_1^{\dagger} + a_2^{\dagger}$  and  $B_{2,2}^{\dagger} = a_1^{\dagger} a_2^{\dagger}$  are elementary symmetric polynomials in the creation operators. For fixed boson number  $n$ , the dimension of  $V_{2,S}$  is  $\text{Dim}(V_{2,S}) = [n/2] + 1$ , where  $[x]$  denotes the integer part of  $x$ . In the large- $n$  limit, this approaches one half of the full  $n$ -boson Hilbert-space dimension  $\text{Dim}(V_{2,n}) = n + 1$ . Consequently, the eigenstates of the dimer Hamiltonian restricted to  $V_{2,S}$  may be written, up to normalization, as

$$|\zeta, n; [1, 2]\rangle = \sum_{\mu=0}^{[n/2]} c_{\mu}^{(\zeta)} B_{2,1}^{\dagger n-2\mu} B_{2,2}^{\dagger \mu} |0\rangle = \sum_{\mu=0}^{[n/2]} c_{\mu}^{(\zeta)} \sum_{\tau=\mu}^{n-\mu} \frac{(n-2\mu)!}{(n-\tau-\mu)!(\tau-\mu)!} a_1^{\dagger n-\tau} a_2^{\dagger \tau} |0\rangle, \quad (\text{B1})$$

where  $[1, 2]$  denotes the two-box Young tableau associated with the totally symmetric irrep of  $S_2$  in the standard  $S_2 \supset S_1$  (Yamanouchi) basis,  $c_{\mu}^{(\zeta)}$  are expansion coefficients determined from diagonalization, and  $B_{2,1}^{\dagger n-2\mu} B_{2,2}^{\dagger \mu} |0\rangle$  form a complete basis of  $S_2$ -symmetric  $n$ -boson states.

For the trimer, the basis vectors spanning the totally symmetric subspace  $V_{3,S}$ , associated with the  $[3, 0]$  irrep of  $S_3$ , may be expressed as  $B_{3,1}^{\dagger n-2\mu_1-3\mu_2} B_{3,2}^{\dagger \mu_1} B_{3,3}^{\dagger \mu_2} |0\rangle$ , where  $B_{3,1}^{\dagger} = a_1^{\dagger} + a_2^{\dagger} + a_3^{\dagger}$ ,  $B_{3,2}^{\dagger} = a_1^{\dagger} a_2^{\dagger} + a_1^{\dagger} a_3^{\dagger} + a_2^{\dagger} a_3^{\dagger}$ , and  $B_{3,3}^{\dagger} = a_1^{\dagger} a_2^{\dagger} a_3^{\dagger}$  are the elementary symmetric polynomials in the three creation operators. The dimension of  $V_{3,S}$  is  $\text{Dim}(V_{3,S}) = \text{Round}[n(n+6)/12 + (7 + (-1)^n)/8 - \sqrt{12} |\sin \frac{n}{3}|/9]$ , where  $\text{Round}[x]$  denotes the nearest integer. In the large- $n$  limit,  $\text{Dim}(V_{3,S}) \sim n^2/12$  and  $\text{Dim}(V_{3,M}) \sim n^2/3$ .

Using the induction  $S_2 \otimes S_1 \uparrow S_3$  [36], the basis vectors of the totally symmetric irrep  $[3, 0, 0]$  and the mixed-symmetry irrep  $[2, 1, 0]$  of  $S_3$  can be expressed in terms of  $S_2 \otimes S_1$  basis vectors as follows:

$$|[1, 2, 3]\rangle = \sqrt{\frac{1}{3}} (|[1, 2]; 3\rangle + |[1, 3]; 2\rangle + |[2, 3]; 1\rangle), \quad (\text{B2})$$

$$\left| \begin{smallmatrix} 1, 2 \\ 3 \end{smallmatrix} \right\rangle = -\sqrt{\frac{2}{3}} |[1, 2]; 3\rangle + \sqrt{\frac{1}{6}} |[1, 3]; 2\rangle + \sqrt{\frac{1}{6}} |[2, 3]; 1\rangle, \quad (\text{B3})$$

$$\left| \begin{smallmatrix} 1, 3 \\ 2 \end{smallmatrix} \right\rangle = -\sqrt{\frac{1}{2}} |[1, 3]; 2\rangle + \sqrt{\frac{1}{2}} |[2, 3]; 1\rangle, \quad (\text{B4})$$

where  $[i, j]$  and  $[i, j, k]$  ( $i < j < k$ ) denote the totally symmetric irreps of  $S_2$  and  $S_3$ , respectively, in the standard Young-tableau basis.

Suppose that  $|\eta, n; [1, 2]; 3\rangle$  is an  $S_2$ -symmetric eigenstate of the trimer Hamiltonian, satisfying

$$\hat{H}_3 |\eta, n; [1, 2]; 3\rangle = E_n^{(\eta)} |\eta, n; [1, 2]; 3\rangle. \quad (\text{B5})$$

The corresponding  $S_3$ -symmetric eigenstate with the same eigenvalue is obtained through symmetrization according to

$$|\eta, n; [1, 2, 3]\rangle = \sqrt{\frac{1}{3}} (1 + (2, 3) + (1, 2)(2, 3)) |\eta, n; [1, 2]; 3\rangle, \quad (\text{B6})$$

provided it is nonvanishing, where  $(i, i+1)$  with  $1 \leq i \leq 2$  denotes the site  $i$  and  $i+1$  permutation. Otherwise, the eigenstate belongs to the mixed-symmetry irrep  $[2, 1, 0]$  and is generated by

$$\left| \eta, n; \begin{smallmatrix} 1, 2 \\ 3 \end{smallmatrix} \right\rangle = \left( -\sqrt{\frac{2}{3}} + \sqrt{\frac{1}{6}} (2, 3) + \sqrt{\frac{1}{6}} (1, 2)(2, 3) \right) |\eta, n; [1, 2]; 3\rangle. \quad (\text{B7})$$

Because the Hamiltonian is invariant under the full permutation group  $S_3$ , states belonging to different irreps are orthogonal and may possess different eigenvalues.

The eigenstates of  $\hat{H}_3$ ,  $|\eta, n; [1, 2]; 3\rangle$ , can be expressed as

$$|\eta, n; [1, 2]; 3\rangle = \sum_{\mu_1=0}^{[n/2]} \sum_{\mu_2=0}^{n-2\mu_1} c_{\mu_1, \mu_2}^{(\eta)} B_{2,1}^{\dagger n-2\mu_1-\mu_2} B_{2,2}^{\dagger \mu_1} a_3^{\dagger \mu_2} |0\rangle, \quad (\text{B8})$$

where  $c_{\mu_1, \mu_2}^{(\eta)}$  is the expansion coefficient determined from diagonalization. According to Eqs. (B5), (B6), and (B7), the eigenstates shown in Eq. (B8) belong to the subspace  $V_{3,S} \oplus V_{3,M}$ . Since Eq. (B8) is  $S_2$  symmetric, the eigenstates shown in Eq. (B8) are those of Eqs. (B6) and (B7). Thus, the total number of eigenstates provided by Eq. (B8) is given by  $\dim(V_{3,S}) + \dim(V_{3,M})/2$ .

Mathematica codes for diagonalizing the dimer and trimer BHM Hamiltonians in the  $S_2$  symmetric subspace according to Eqs. (B1) and (B8) are provided in the Supplemental Material [38].

Alternatively, the recursive construction of trimer eigenstates from dimer eigenstates can also be implemented within a permutation-symmetry-adapted basis. For the trimer Hamiltonian (2) with  $p = 3$ , the eigenstates belonging to the subspace of dimension  $\dim(V_{3,S}) + \dim(V_{3,M})/2$  may be expanded in terms of the  $S_2$ -symmetric dimer eigenstates as

$$|\eta, n; [1, 2]; 3\rangle = \sum_{k=0}^n \sum_{\zeta=1}^{[(n-k)/2]+1} Z_{\zeta, k}^{(SM; \eta)} a_3^{\dagger n-k} |\zeta, k; [1, 2]\rangle, \quad (\text{B9})$$

where  $Z_{\zeta, k}^{(SM; \eta)}$  are expansion coefficients to be determined and  $|\zeta, k; [1, 2]\rangle$  are the dimer eigenstates in the  $S_2$ -symmetric subspace given by Eq. (B1). The eigenvalue equations determining  $E_n^{(\eta)}$  and  $Z_{\zeta, k}^{(SM; \eta)}$  have the same form as Eqs. (18)–(21), except that the transfer amplitudes  $\Lambda_{\zeta' \zeta}^{2, k}$  are replaced by the symmetry-adapted matrix elements  $\Lambda_{\zeta' \zeta}^{\text{Sym}, k}$ ,

$$\Lambda_{\zeta' \zeta}^{\text{Sym}, k} = \frac{\langle \zeta', k; [1, 2] | (a_1 + a_2) | \zeta, k + 1; [1, 2] \rangle}{\sqrt{\langle \zeta', k; [1, 2] | \zeta', k; [1, 2] \rangle \langle \zeta, k + 1; [1, 2] | \zeta, k + 1; [1, 2] \rangle}}, \quad (\text{B10})$$

with

$$\begin{aligned} \langle \zeta', k; [1, 2] | (a_1 + a_2) | \zeta, k + 1; [1, 2] \rangle &= \sum_{\mu=0}^{[k/2]} \sum_{\mu'=0}^{[(k+1)/2]} \sum_{\tau=\max(\mu, \mu')}^{\min(k+1-\mu', k+1-\mu)} c_{\mu}^{(\zeta')} c_{\mu'}^{(\zeta)} \\ &\times \frac{(k+1-2\mu)! (k+1-2\mu')! (k+1-\tau)! \tau!}{(k+1-\tau-\mu)! (k+1-\tau-\mu')! (\tau-\mu)! (\tau-\mu')!} \end{aligned} \quad (\text{B11})$$

and

$$\begin{aligned} \langle \zeta, k; [1, 2] | \zeta, k; [1, 2] \rangle &= \sum_{\mu=0}^{[k/2]} \sum_{\mu'=0}^{[k/2]} \sum_{\tau=\max(\mu, \mu')}^{\min(k-\mu', k-\mu)} c_{\mu}^{(\zeta)} c_{\mu'}^{(\zeta)} \\ &\times \frac{(k-2\mu)! (k-2\mu')! (k-\tau)! \tau!}{(k-\tau-\mu)! (k-\tau-\mu')! (\tau-\mu)! (\tau-\mu')!}. \end{aligned} \quad (\text{B12})$$

The normalization factors in the denominator of Eq. (B10) are required because the basis states (B1) are not normalized. Consequently, the recursive formalism can be implemented directly in a symmetry-adapted representation, combining the dimensional reduction provided by permutation symmetry with the sparse near-tridiagonal structure generated by the recursive construction.

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