

Zero-point energy of tensor fluctuations on the matrix product state manifold

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This work presents a method to quantize low energy excitations of systems whose ground state is best represented by a matrix product state (MPS) such as the Affleck-Kennedy-Lieb-Tasaki (AKLT) model. The approach is similar to the spin-wave model of excitations in typical magnetic materials, but includes a more general set of fluctuations in entanglement structure. We argue that the quasilocal action of tensor fluctuations facilitates a description in terms of bosonic modes. We apply this approach to compute fluctuation corrections to the bilinear-biquadratic Heisenberg model, whose ground state we expect to be close to the exact bond dimension 2 AKLT state in a certain parameter range. Our results show significant improvements in energy approximations, highlighting both the qualitative and quantitative potential of this paradigm for studying complex entangled systems. This approach paves the way for new insights into the low-energy physics of correlated materials and the development of effective field theories beyond traditional semiclassical methods.

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Introduction. The theory of spin waves, first introduced by Bloch [1], is a very important tool for understanding low-temperature magnetic materials. It consists of assuming an ordered product state background whose excitations are described by propagating fluctuations of the spin direction, which are modeled using bosonic modes via the Holstein-Primakoff transformation [2]. This has been extremely effective in explaining a range of phenomena in quantum systems with ferromagnetic and antiferromagnetic orderings [3–7], including the dressing of magnetic ground states by zero-point fluctuations.

More recently, tensor networks have been among the most widely used tools in condensed matter theory [8–10], giving rise to numerous theoretical results such as the classification of possible phases of matter in 1D [11], as well as unmatched numerical accuracy in tasks such as ground-state approximation [12–15]. The proliferation of these techniques stems from the ability to represent area-law entanglement patterns using only polynomially many parameters, which is enough to faithfully represent the ground state of gapped local Hamiltonians in 1D. Despite their success, understanding the low-energy physics of such systems is still an area of active research. Global quench dynamics is expected to thermalize in most systems, leading to volume law entanglement and a breakdown of the matrix product state representation. Several techniques have been proposed to address this issue and gain insight into low-energy physics, such as tensor network based variational ansatz for understanding excitation spectra

[16–19] and the truncation of operator entanglement for computing transport properties [20].

We propose a method for understanding low-energy physics based on an adaptation of spin-wave treatment to magnetic systems whose ground states have complex entanglement patterns, such as the $S = 1$ Affleck-Kennedy-Lieb-Tasaki (AKLT) model [21]. The low-energy physics is still governed by propagating fluctuations treated as independent bosonic modes, but the local disturbance can be any variation in the tensor structure.

Understanding the MPS double tangent space, as introduced and studied in previous works [22,23], was fundamental to this research. The configuration interaction with single and double excitations (CISD) ansatz for approximating ground states was discussed earlier in [24], where the generalized eigenvalue equation in the redundant space of single and double tangent space vectors was constructed and solved numerically. Previous work [25] attempted to subsume these ideas into a field-theoretical framework by constructing a path integral on the MPS manifold. Expanding about the saddles of this theory suggested a bosonic interpretation for the CISD equation and derived an effective Hamiltonian for the excitations. The normal part is identical to that used in the excitation ansatz [16], but it additionally includes anomalous terms accounting for production of bosons in pairs. A naive treatment overcounts the number of bosonic states, giving rise to unreasonably large fluctuations. We complete this picture by incorporating the insights of Ref. [26] and explicitly constructing a quasilocal bosonic Gram operator to recover the correct overlaps between the various tangent spaces. The result is an effective geometric quantization of the MPS manifold seen as a classical phase space [27,28]. This approach offers significant technical and philosophical advantages over brute-force optimization methods.

Matrix product states. For a system with N sites and open boundary conditions, we introduce the generic form of a

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matrix product state (MPS) defined via the local three-tensors $\mathcal{A} = \{\mathbf{A}^{[i]}\}_{i=1}^N$ with a physical index of dimension d and two bond indices going up to the bond dimension D . The bond indices are contracted sequentially to produce the matrix product state

$$= \text{---} \bigcirc_{A^{[1]}} \text{---} \bigcirc_{A^{[2]}} \text{---} \dots \text{---} \bigcirc_{A^{[N]}} \text{---} \quad (1)$$

Such constructions are subject to gauge freedom, as any transformation $A^{[i]} \rightarrow A^{[i]}X$, $A^{[i+1]} \rightarrow X^{-1}A^{[i+1]}$ will give rise to the same state. This issue can be resolved without losing expressivity by enforcing a more restrictive parametrization for the tensors at each site. Part of the gauge is fixed by enforcing left-canonical form, which can be obtained from a unitary U in the following way:

Diagrammatic equation (2) shows the equivalence between a circle with $A^{[z]}$ and a square with $U^{[z]}$. The circle has four external legs (top, bottom, left, right). The square has four external legs (top, bottom, left, right) and an additional input from a circle labeled 0 at the top. The equation is labeled (2) on the right.

The remaining gauge freedom is fixed by restricting U to the following parametrized form $U^{[i]}(x) = U \exp(x_i \langle 0| \otimes \Gamma^{1/2} - |0\rangle \otimes \Gamma^{1/2} x_i^\dagger)$. An equivalent version was introduced in [24], alongside a proof that it covers the entire MPS manifold. We give an explicit construction for the x_i parameters in the Supplemental Material [29]. The exponent is given by the $\mathfrak{su}(D \times d)$ algebra element

$- \text{H. c.},$

(3)

where the entries of the $D \times D \times (d - 1)$ tensor x_i are arbitrary complex numbers, and Γ is the right environment. In the following, we will assume translational invariance and finite correlation length ξ .

We will use the Greek letters μ, ν , etc., to index the different entries of x_i , corresponding to the different ways in which the local tensor can fluctuate. The advantage of this choice lies in having the simple Gram matrix for the vectors in the first tangent space $\langle \partial_\mu^{(i)} \Psi | \partial_\nu^{(j)} \Psi \rangle = \delta_{\mu\nu} \delta_{ij}$ in the thermodynamic limit $N \rightarrow \infty$ [22]. We will call the presence of a derivative on some site a local excitation, as it can be seen that the state $|\partial_\mu^{(i)} \Psi\rangle$ is also an MPS, where the tensor at site i was replaced by a tangent tensor B_μ given by

$$\text{---} \bigcirc B_\mu \text{---} = \text{---} \left[\begin{array}{c} \text{---} \downarrow \text{---} \\ \text{---} \leftarrow \text{---} \end{array} U \begin{array}{c} \text{---} \uparrow \text{---} \\ \text{---} \rightarrow \text{---} \end{array} \left(\text{---} \bigcirc e_\mu \text{---} \right) \left(\text{---} \bigcirc \Gamma^{-\frac{1}{2}} \text{---} \right) \text{---} , \quad (4)$$

where e_μ is a unit tensor with a 1 in position μ and 0 elsewhere. Vectors spanning higher tangent spaces can be obtained by taking derivatives at different sites.

Bosonic mapping. In the following section we will argue that the local perturbations of the reference MPS can be understood via a set of bosonic modes. These excitations are produced by taking derivatives of the MPS along different

directions μ at different sites i and can be associated with creation and annihilation operators $a_{\mu}^{(i)\dagger}, a_{\mu}^{(i)}$.

In the case of single excitations the orthonormalization of the single tangent space ensures that the overlaps are identical to those obtained from a bosonic Fock space. In the case of two or more excitations, this identification holds only when the separation is much larger than the correlation length. However, complications arise due to an overcounting of states with excitations separated by small distances. One can see this by noting that the basis formed by taking derivatives will have $(1 + D^2(d - 1))^N$ states, corresponding to placing either an A tensor or one of the B_μ tensors at each site. If $D > 1$, this will be larger than d^N , the dimension of the physical Hilbert space, indicating redundancy in the bosonic framework. It is a direct consequence of the delocalized nature of excitations of entangled reference states and has been noted in other works using tensor networks to represent states with two elementary excitations [30,31].

We give a general construction accounting for these effects for excitations above an MPS reference state. First, we consider the (unnormalized) state $|\partial_\mu^{(i)} \partial_\nu^{(i+x)} \Psi\rangle$ where the separation is large compared to the correlation length of the reference state $x \gg \xi$. We will look at the overlap of this with another two excitation states $|\partial_\alpha^{(j)} \partial_\beta^{(j+y)} \Psi\rangle$. The left canonicalization of the MPS ensures that for a nonzero overlap we need to take the left-most derivatives in the same place, so that $i = j$. If we introduce the notation $T(A, B)$ for the transfer matrix

$$T(A, B) = \begin{array}{c} \text{---} \circ A \text{---} \\ | \\ \text{---} \circ B^* \text{---} \end{array}, \quad (5)$$

and the transfer matrix of the reference state $T(A, A) = T$, we see that the overlap between the states with $y < x$ is

$$\begin{aligned} & \langle \partial_\alpha^{(i)} \partial_\beta^{(i+y)} \Psi | \partial_\mu^{(i)} \partial_\nu^{(i+x)} \Psi \rangle \\ &= (I | T(B_\mu, B_\alpha) T^{y-1} T(A, B_\beta) T^{x-y-1} T(B_\nu, A) | \Gamma), \quad (6) \end{aligned}$$

where we have used the fact that $\lim_{n \rightarrow \infty} T^n = |\Gamma\rangle\langle I|$ and follow the notation of Ref. [22] for states in the doubled auxiliary space. When $x \gg \xi$, one of the two powers of the transfer matrix in the above expression will be close to its limit at infinity, which is null since $\langle I|T(A, B_\mu) = 0$ by the definition of the tangent space tensors. The overlap above must then be of order $\mathcal{O}(e^{-x/\xi})$. When the right-most excitations overlap, we have instead

$$\begin{aligned} & \langle \partial_\alpha^{(i)} \partial_\beta^{(i+x)} \Psi | \partial_\mu^{(i)} \partial_v^{(i+x)} \Psi \rangle \\ &= (I | T(B_\mu, B_\alpha) T^{x-1} T(B_v, B_\beta) | \Gamma) \\ &\approx (I | T(B_\mu, B_\alpha) | \Gamma) (I | T(B_v, B_\beta) | \Gamma) = \delta_{\mu\alpha} \delta_{v\beta}, \quad (7) \end{aligned}$$

which is the same as we would expect from bosonic excitations, up to the small error which is exponentially suppressed in the distance. This argument allows us to break overlaps into clusters whenever there is a separation much larger than ξ . When the excitations are located close together, the argument fails and we need to account for the deviations from bosonic overlaps.

In order to deal with the nontrivial overlaps of nearby excitations, we introduce the Gram operator $\mathcal{G}$, which we define such that

$$\left\langle \prod_{\mu,i} \partial_{\mu}^{(i)} \Psi \middle| \prod_{\nu,j} \partial_{\nu}^{(j)} \Psi \right\rangle = [GS] \prod_{\mu,i} a_{\mu}^{(i)} \mathcal{G} \prod_{\nu,j} a_{\nu}^{\dagger(j)} [GS], \quad (8)$$

for all possible sets of positions and directions of the excitations (restricted to a single excitation per site). The notation $[\cdot]$ is used to distinguish states in the bosonic space from those in the physical Hilbert space, with a more detailed construction given in the Supplemental Material [29]. We can expand the Gram operator as a normally ordered polynomial of the creation and annihilation operator, with the argument above guaranteeing that each monomial either has no gaps larger than $\sim \xi$ or is exponentially suppressed. After performing a change of coordinates such as to remove the overlap between the first and second tangent spaces (details in the Supplemental Material [29]), the Gram operator can be expanded as

$$\mathcal{G} = 1 + \sum_{\substack{\mu\nu\alpha\beta, i \\ x, y > 0}} g_{\mu\nu\alpha\beta}^{(xy)} a_{\mu}^{(i)\dagger} a_{\nu}^{(i+x)\dagger} a_{\alpha}^{(i)} a_{\beta}^{(i+y)} + \dots, \quad (9)$$

where g becomes exponentially small for large x or y . The Gram operator also encodes constraints related to which excitations are allowed to be near each other. This is because $\mathcal{G}$ is not full rank, so there are two-excitation states of zero norm under $\mathcal{G}$. On the other hand, some two-excitation states obtain much larger norms than would be predicted by the bosonic analogy, giving rise to the overcounting factor discovered in an earlier work [26].

Operators. In this section we will discuss two approaches for obtaining the bosonic representation of some operator acting on the physical space. Such representations are similar to the Holstein-Primakoff transformation, with two important distinctions. Here, the expansion of an operator at site i is only quasilocal, with contributions from bosonic operators located at sites to the right of i . Second, for a faithful representation we need to remove all states of zero norm under the inner product defined in Eq. (8). A rigorous introduction to the mapping is given in the Supplemental Material [29].

We will mainly refer to the Hamiltonian H , but the same construction holds for any operator of interest. The first method is based on tensor network contractions and has been used by Haegeman *et al.* [16] to compute dispersion relations. We look for a quadratic approximation to the Hamiltonian of the form

$$H_B = E_0 + \sum_{i\mu\nu} \epsilon_{\mu\nu}^{(x)} a_{\mu}^{(i)\dagger} a_{\nu}^{(i+x)} + \sum_{i\mu\nu} \Delta_{\mu\nu}^{(x)} a_{\mu}^{(i)\dagger} a_{\nu}^{\dagger(i+x)} + \overline{\Delta}_{\mu\nu}^{(x)} a_{\mu}^{(i)} a_{\nu}^{(i+x)}. \quad (10)$$

The idea is to relate the coefficients in the expansion to the matrix elements of the physical Hamiltonian in the basis of tangent space vectors

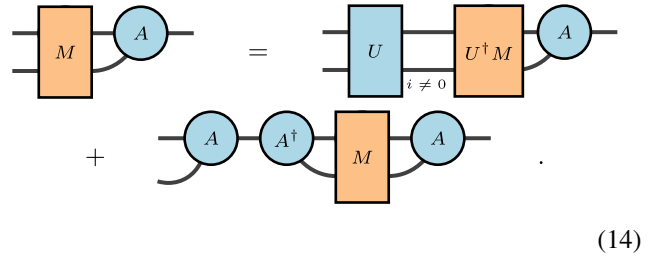
$$E_0 = \langle \Psi | H | \Psi \rangle, \quad (11)$$

$$\epsilon_{\mu\nu}^{(ij)} = \langle \partial_{\mu}^{(i)} \Psi H | \partial_{\nu}^{(j)} \Psi \rangle - E_0 \delta_{\mu\nu} \delta_{ij}, \quad (12)$$

$$\Delta_{\mu\nu}^{(ij)} = \langle \partial_{\mu}^{(i)} \partial_{\nu}^{(j)} \Psi | H | \Psi \rangle. \quad (13)$$

The Gram matrix is not the identity in the second tangent space, so these coefficients correspond to the quadratic terms of the operator $H'_B = \mathcal{G} H_B$ rather than H_B . The normal part is unaffected by this distinction, and gives rise to the same dispersion relations in [16]. The annihilation part remains unaltered, so $\overline{\Delta} = \Delta'^*$, but using Δ' for the pair production term leads to too many excitations, since the vectors $|\partial_{\mu}^{(i)} \partial_{\nu}^{(j)} \Psi\rangle$ are not linearly independent. To obtain the correct Δ one needs to apply the inverse of the Gram matrix, which is explained further in the Supplemental Material [29].

The second method builds the Hamiltonian H_B directly by looking at how the terms in the Hamiltonian interact with the structure of the local tensors of the MPS. To see how this works, consider some matrix M that acts on both the physical and the bond indices of the output of tensor A . The pull-through equation consists of writing this tensor as a linear combination of a local derivative and a term with a matrix on the opposite side of A . This can be expressed diagrammatically as



$$\text{Diagrammatic equation (14): } M \text{ acting on } A = U \text{ acting on } A + A^\dagger M \text{ acting on } A. \quad (14)$$

The first term on the RHS is a local derivative term parametrized by the three-tensor $x = (1 - |0\rangle \langle 0|_p) U^\dagger M A \sqrt{\Gamma}$ [compare with Eq. (4)]. In the second term M has been “pulled through” to the other side of the local tensor A . This equation can be applied recursively to move M to the right end of the chain. The properties of the transfer matrix governing the pull-through map $M \rightarrow A^\dagger M A$ guarantee that all terms decay exponentially quickly, except for the identity. The same principle holds for pulling matrices through derivative tensors, with the details found in the Supplemental Material [29]. If we apply this procedure to initial operators h acting in the physical space, we end up with a mapping similar to the Holstein-Primakoff transformation from the set of single-site physical operators h to the bosonic space. This approach does not automatically remove zero-norm two-particle states, so these must be projected out after constructing the quasiparticle Hamiltonian. Once this is accounted for, the two methods produce the same Hamiltonian.

Fluctuation correction. To illustrate the power of our approach we consider an example task of calculating the fluctuation corrections to the ground state energy. This is equivalent to solving the following minimization equation:

$$E = \min_{\phi} \frac{[\phi | \mathcal{G} H_B | \phi]}{[\phi | \mathcal{G} | \phi]}, \quad (15)$$

where $|\phi\rangle$ is a bosonic state. This leads to the generalized eigenvalue equation

$$\mathcal{G} H_B |\phi\rangle = E \mathcal{G} |\phi\rangle, \quad \mathcal{G} |\phi\rangle \neq 0 \quad (16)$$

which is complicated by the fact that $\mathcal{G}$ is not invertible due to the zero-norm states discussed previously. This is equivalent

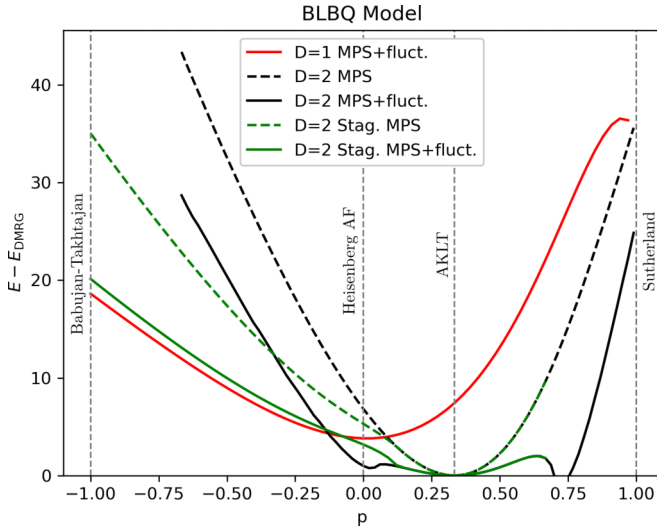


FIG. 1. Ground state energy approximations for the BLBQ model of Eq. (17) in the Haldane phase corresponding to the parameter p in the range -1 – 1 . The energy surplus is compared to a $\chi = 50$ DMRG. The $D = 1$ and the $D = 2$ Stag. results are obtained by applying a flip on every other site. Dashed lines mark single MPS results and bold lines include fluctuation corrections.

to solving the regular eigenvalue problem for $\mathcal{G}^+ \mathcal{G} H_B$, where $\mathcal{G}^+$ is the pseudoinverse. Then we can proceed with the usual spin-wave treatment, by truncating the operator at quadratic order and computing the ground state energy and excitation spectrum via a Bogoliubov transformation [32].

Results. We test the algorithm described above for computing fluctuation corrections of the following set of parametrized spin-1 Hamiltonians,

$$\mathcal{H} = \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + p(\vec{S}_i \cdot \vec{S}_{i+1})^2, \quad (17)$$

called the isotropic bilinear-biquadratic (BLBQ) Heisenberg model [33–35]. This is known to be in the Haldane phase for p between -1 and 1 , which includes the Heisenberg antiferromagnet at $p = 0$ and the AKLT model at $p = 1/3$. The reason for this choice is that the ground state of the AKLT model is exactly an MPS with $D = 2$. It also remains a saddle point of the TDVP equations for a wider range of θ values in the same phase, forming a good reference state. Its transfer matrix is simple, allowing us to gain analytical insight into the structure of Gram operators, with details in the Supplemental Material [29]. The fluctuation corrections to the ground state energy at various values of the parameter p are shown in Fig. 1. We observe significant improvements in the region around the AKLT $p = 1/3$.

We also check how the performance of the algorithm is affected by the choice of bond dimension. For this purpose, we consider both the spin-1 BLBQ model described above with $\Delta p = 0.3 = p - p_{\text{AKLT}}$, as well as the spin-1/2 Heisenberg model with an applied staggering field $h = 0.2$ to remove ground state degeneracy. For the latter, the $D = 1$ calculation matches the typical Holstein-Primakoff quadratic approximation. The first thing we note is that the free particle fluctuation correction constitutes the largest fraction of the remaining energy at the lowest bond dimension that allows

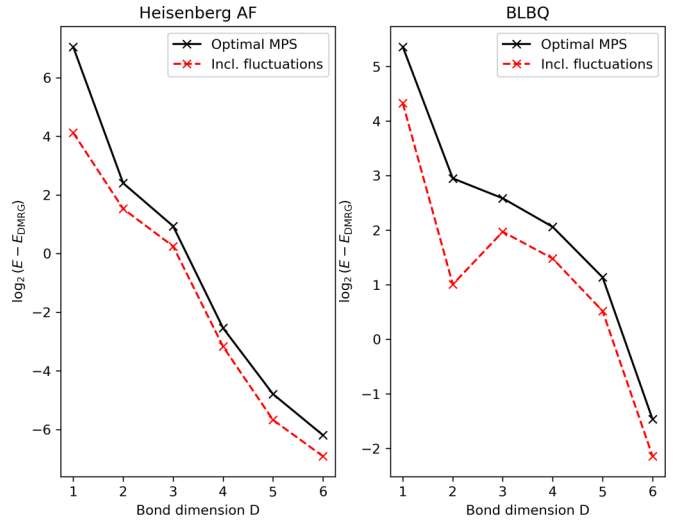


FIG. 2. Energy at various bond dimensions with and without zero-point fluctuation energy, compared to a $\chi = 50$ DMRG. Left panel is for the $S = 1/2$ Heisenberg antiferromagnet with an applied staggered magnetic field. Right panel is for the $S = 1$ BLBQ model with a particular choice of $p = p_{\text{AKLT}} + 0.3$.

for a qualitatively correct reference state. For the Heisenberg antiferromagnet this is the $D = 1$ Néel state, while the BLBQ model is in the Haldane phase, which is qualitatively similar to the $D = 2$ AKLT state. In the BLBQ case, the plot of energies including fluctuations is not strictly decreasing as one may expect, showing that the second tangent spaces around the variational minimum at different bond dimensions do not form strictly increasing sets. As the bond dimension is increased beyond this point, we find that the fluctuation correction approaches a finite fraction of the gap, which is represented by a nearly constant distance between the graphs in Fig. 2. This suggests a perturbative treatment of the interactions may be easiest by working on the lowest bond dimension manifold that is able to qualitatively capture the entanglement structure of the true ground state.

Discussion. We presented a method for constructing a bosonic representation of tensor fluctuations around an MPS reference point. This can be understood as a generalization of the Holstein-Primakoff transformation for treating complex systems where primary excitations are delocalized over multiples sites. We illustrate the method by constructing the effective quadratic bosonic Hamiltonian of the BLBQ model inside the Haldane phase, where the AKLT ground state is a good reference. We showed that the fluctuation correction due to the pairing of AKLT spinons is well behaved and accounts for a large portion of the distance to the energy of the true ground state. Due to the simplicity associated with free boson theories and our method for constructing bosonic equivalents for arbitrary spin operators, corrections to a large number of observables of interest could also be obtained. We do not discuss topological excitations or nontranslationally invariant reference states here, but we expect they can be included in a similar fashion, at the expense of dealing with more complicated Gram operators. Additionally, the same methodology could be used to compute fluctuation corrections above PEPS, starting from the dispersion relations computed in [18].

The effect of both the bosonic Hamiltonian and the Gram operator could be captured by a path integral over the MPS manifold, which has been previously proposed [25]. In this formulation, the Gram operator appears as a local fourth order modification to the bosonic Berry phase, which has been shown here and in previous work [26] to contribute meaningfully at the free boson level of approximation. A more thorough investigation of this connection and its implications for constructing path integrals over entangled phase spaces is left for future work. Combined with renormalization group methods, this approach could lead to effective field theories of phase transitions beyond those accessible by the Landau-Ginzburg mean-field approach.

Finally, we remark that our work could prove a very effective theoretical tool for studying exotic materials, by systematically constructing tensor approximations to local excitations along with their interaction Hamiltonian. Constructing the effective Hamiltonian to higher orders is straightforward in principle by following the pull-through

equations detailed in the Supplemental Material [29]. The dynamics obtained are expected to produce important insights and more accurate low-energy descriptions that can be used to better understand the physics behind phase transitions and higher-dimensional systems beyond the reach of standard tensor network simulations. Once the Gram operator for a certain reference state is understood, the process of including interactions perturbatively follows in a similar way to standard spin-wave treatments. It is exciting to speculate that the principles outlined here could eventually be used to automate the identification and classification of key low-energy physics and to propose effective field theories for their excitations.

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Data availability. The data that support the findings of this study are available from the corresponding author upon request.

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