

Combined use of translational and spin-rotational invariance for spin systems

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Exact diagonalization and other numerical studies of quantum spin systems are notoriously limited by the exponential growth of the Hilbert space dimension with system size. A common and well-known practice to reduce this increasing computational effort is to take advantage of the translational symmetry C_N in periodic systems. This represents a rather simple yet elegant application of the group theoretical symmetry projection operator technique. For isotropic exchange interactions, the spin-rotational symmetry $SU(2)$ can be used, where the Hamiltonian matrix is block-structured according to the total spin- and magnetization quantum numbers. Rewriting the Heisenberg Hamiltonian in terms of irreducible tensor operators allows for an efficient and highly parallelizable implementation to calculate its matrix elements recursively in the spin-coupling basis. When combining both C_N and $SU(2)$, mathematically, the symmetry projection technique leads to ready-to-use formulas. However, the evaluation of these formulas is very demanding in both computation time and memory consumption, problems which are said to outweigh the benefits of the symmetry reduced matrix shape. We show a way to minimize the computational effort for selected systems and present the largest numerically accessible cases.

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I. INTRODUCTION

A typical system that possesses both spin-rotational as well as translational symmetry is a Heisenberg spin ring^{1–19} which models, e.g., certain magnetic molecules or chains with the following Hamiltonian, where periodic boundary conditions are applied,

$$\hat{H} = -2J \sum_{i=1}^N \vec{s}_i \cdot \vec{s}_{i+1}, \quad \vec{s}_{N+1} \equiv \vec{s}_1. \quad (1)$$

The dot-product between the spin vector operators ensures spin rotational symmetry, since dot-products do not change upon simultaneous rotations of both vectors. The same value J of interactions between adjacent neighbors gives rise to translational invariance, since the spin ring can be collectively moved by one spacing without changing the Hamiltonian.

Both symmetries can be employed for various purposes. One is of course the perception of fundamental properties without even evaluating the energy spectrum: the energy eigenvalues form multiplets, i.e. total spin S and its magnetic quantum number M are good quantum numbers. The same holds for the momentum quantum number $k = 0, \dots, N-1$, that also explains certain degeneracies, namely between k and $N-k$.^{7,20–24} Together with the notion of bipartiteness these quantum numbers can be assigned to, for instance, the ground state, again without diagonalizing the Hamiltonian.^{25–27}

The other application is the reduction of dimensionality when diagonalizing the Hamiltonian. This is achieved by block-structuring the Hamiltonian matrix according to the available quantum numbers, or in the language of group theory, the available irreducible representations. This powerful tool, that is heavily used in exact diagonalization studies, is the topic of this investigation. In order

to guide the reader to the achievements and problems of combining full spin-rotational symmetry with translational symmetry, we present important precursors first.

For spin problems, where at least the total magnetization M is a good quantum number, i.e. $[\hat{H}, \hat{S}^z] = 0$, one can subdivide the full Hilbert space \mathcal{H} into the direct sum of all eigenspaces $\mathcal{H}(M)$ of \hat{S}^z

$$\mathcal{H} = \bigoplus_{M=-S_{\max}}^{+S_{\max}} \mathcal{H}(M). \quad (2)$$

This is easily achieved by sorting the product basis states $|m_1, m_2, \dots, m_N\rangle$ according to their total magnetic quantum number $M = \sum_{i=1}^N m_i$, which yields basis states $|m_1, m_2, \dots, m_N; M\rangle$ in each orthogonal subspace $\mathcal{H}(M)$.²⁸ This scheme is employed in many popular codes for exact and approximate diagonalization, as for instance, by means of Density Matrix Renormalization Group (DMRG), compare, e.g., the ALPS package.^{29,30}

To marry the \hat{S}^z -symmetry with translational symmetry is again rather easy since the irreducible representations of the translations can be constructed analytically starting from states $|m_1, m_2, \dots, m_N; M\rangle$. If \hat{T} denotes a translation of the chain by one site, i.e. the generating group operation of the translation group C_N , then

$$|m_1, m_2, \dots, m_N; M, k\rangle \propto \sum_{\nu=0}^{N-1} \left(e^{i2\pi k/N} \hat{T} \right)^\nu |m_1, m_2, \dots, m_N; M\rangle \quad (3)$$

is both an eigenstate of \hat{S}^z and \hat{T} with eigenvalues M and $\exp(-i2\pi k/N)$, respectively, $k = 0, \dots, N-1$ being the shift quantum number (lattice momentum). After considering that cyclic permutations of m_1, m_2, \dots, m_N

yield the same $|m_1, m_2, \dots, m_N; M, k\rangle$ and that some patterns m_1, m_2, \dots, m_N with additional symmetry do contribute only to certain k , one can set up a very straight forward generation of the basis states in the subspaces $\mathcal{H}(M, k)$, whose dimensions are about $1/N$ th of the respective dimensions of $\mathcal{H}(M)$.^{7,31–34} This scheme is also used in many programs, among which `spinpack` is a freely available one.³⁵ Application in DMRG seems to be restricted since matrix-product states are constructed according to positions of spins, therefore each state breaks translational invariance. Nevertheless, very recently ideas have been developed how to incorporate translational symmetry into DMRG.³⁶

Then, what is the problem with the combination of full spin-rotational symmetry and translational symmetry?

The paper is organized as follows. In Section II we recapitulate how spin rotational and translational symmetry can be applied simultaneously and discuss the numerical implications. Thereafter in Section III we present some of the largest numerically exact calculations for spin rings followed by a discussion in Section IV.

II. SPIN-ROTATIONAL AND TRANSLATIONAL SYMMETRY

The major obstacle when combining spin-rotational and translational symmetry is given by the fact, that a translated eigenstate of \tilde{S}^2 in general does not belong to the same basis set as the original state, in contrast to the basis $\{|m_1, m_2, \dots, m_N; M\rangle\}$, where translations yield just another member of the same basis set. In order to understand this better, we quickly repeat how spin-rotational symmetry – $SU(2)$ – can be realized. This is done by means of spin coupling according to some arbitrary coupling scheme. The basis states

$$|s_1, s_2, S_{12}, s_3, S_{123}, \dots, s_N, S, M\rangle \quad (4)$$

are e.g. generated by sequential coupling of spins along the chain. They are by construction eigenstates of \tilde{S}^2 and \tilde{S}^z . If the Hamiltonian is then written in terms of irreducible tensor operators that are connected to compound tensors according to the same coupling scheme, matrix elements of the Hamiltonian can be easily evaluated by recursive decoupling. A detailed description of this powerful method can be found in references 37–44. The computer program `MAGPACK`, that completely diagonalizes the Heisenberg Hamiltonian using $SU(2)$ symmetry, is freely available.⁴⁵ Also for DMRG $SU(2)$ codes have been developed.^{46–51} In other fields such as nuclear physics this method was also adapted to model finite Fermi systems such as nuclei⁵² as was the case for Hubbard models, where one can actually exploit two $SU(2)$ symmetries.^{53–56} Solutions for models with $SU(N)$ symmetry work along similar lines.^{46,57–60}

The construction of a new basis that is in addition an eigenbasis of the translation operator \tilde{T} involves the

projection operator already introduced in (3),

$$|\alpha, S, M, k\rangle \propto \sum_{\nu=0}^{N-1} \left(e^{i2\pi k/N} \tilde{T} \right)^\nu |\alpha, S, M\rangle. \quad (5)$$

Here α is now a short-hand notation for the full coupling scheme $s_1, s_2, S_{12}, s_3, S_{123}, \dots, s_N$. To be used as a basis, the states $|\alpha, S, M, k\rangle$ still need to be orthonormalized. The application of \tilde{T} in (5) generates a plethora of new states that belong to *different* coupling schemes, i.e. to *different* basis sets. Figure 1 demonstrates the action of \tilde{T} on a coupling scheme of a ring of four spins. The translation of all spins by one unit modifies the whole coupling scheme, which is in stark contrast to the action on product states $|m_1, m_2, \dots, m_N\rangle$, where only a new member of the same basis set is produced.

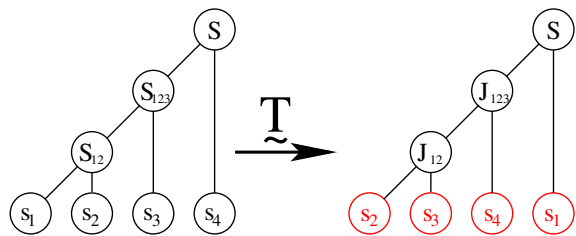


Figure 1. (Color online) Coupling schemes can be represented as coupling trees. The original sequential coupling (l.h.s.) is transformed into a sequential coupling that starts with the spin at position 2 (r.h.s.). The intermediate spins are labeled with a different letter to denote the different coupling scheme, although they acquire the original value, i.e. $J_{12} = S_{12}$.

In order to evaluate matrix elements of the Hamiltonian each state $\tilde{T}^\nu |\alpha, S, M\rangle$ has to be represented in the original basis, i.e.

$$\begin{aligned} \tilde{T}^\nu |\alpha, S, M\rangle = \\ \sum_{\alpha'} |\alpha', S, M\rangle \langle \alpha', S, M | \tilde{T}^\nu |\alpha, S, M\rangle. \end{aligned} \quad (6)$$

Thanks to symmetry this needs to be done only for e.g. $M = S$, but it nevertheless involves a huge number of so-called recoupling coefficients $\langle \alpha', S, M = S | \tilde{T}^\nu |\alpha, S, M = S\rangle$. Graph-theoretical methods can be used to evaluate these coefficients,^{43,44,61,62} which contain Wigner-6J symbols, phase factors, square roots as well as possibly summations over additional indices. The composition of these coefficients is crucial for the computational costs of not only their calculation but also the time and memory efficiency of the whole basis symmetrization. Defining an equivalence relation

$$\begin{aligned} |\alpha', S, M\rangle \cong |\alpha, S, M\rangle \\ \Leftrightarrow \exists \nu : \langle \alpha', S, M | \tilde{T}^\nu |\alpha, S, M\rangle \neq 0 \end{aligned} \quad (7)$$

enables to distinguish orthogonal sets of projected states which can be orthonormalized separately. The num-

ber and size of these sets is closely related to the complexity of the recoupling coefficients, where simple coefficients lead to many small sets. In the worst case, where all states are equivalent, orthonormalization becomes cumbersome and one needs to store an order of $[\dim(\mathcal{H}(S, M = S))]^2 / N$ basis coefficients. This prevents a general use even for relatively small systems.

The complexity of the recoupling coefficients depends on several circumstances, in particular the used point group and the employed coupling scheme.^{43,44} The relevant question is therefore, whether coupling schemes exist that are substantially less demanding than others. In an earlier publication it could be shown that if one chooses compatible point groups and coupling schemes, only phase factors appear in the recoupling coefficients.²¹ Since especially low-symmetry groups such as D_2 or D_4 often allow for the construction of an appropriate coupling scheme,^{63–65} we wonder whether also the group of translations C_N can be combined with a clever coupling scheme.

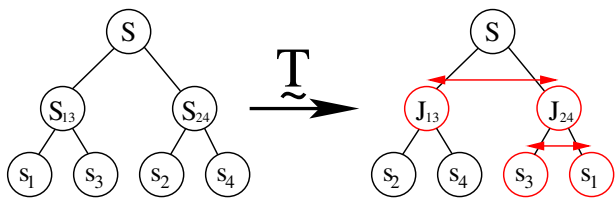


Figure 2. (Color online) Optimal coupling scheme for chain lengths of $N = 2^n$ (l.h.s.). The translated scheme (r.h.s.) can be transformed back into the old coupling scheme by spin exchange operations on the coupling graph, leading to a very simple recoupling coefficient.

The mentioned graph-theoretical methods^{43,44,61,62} help to understand what one is looking for: recoupling coefficients without summations over additional indices and with as few as possible Wigner symbols and square roots. The ultimate goal – no sums, no symbols, no square roots – can be achieved for chain lengths of $N = 2^n, n = 2, 3, 4, \dots$. Then the recoupling coefficients can be evaluated in the graph-theoretical framework by spin exchange processes as depicted in Fig. 2. Such processes generate only a phase, as for example in $\langle s_1 s_2 S | s_2 s_1 S \rangle = (-1)^{S-s_1-s_2}$. For the example shown on the r.h.s. of Fig. 2 this yields ($M = S$ omitted)

$$\begin{aligned} & \langle s_1, s_3, S_{13}, s_2, s_4, S_{24}, S | s_2, s_4, J_{13}, s_3, s_1, J_{24}, S \rangle \\ &= (-1)^{J_{24}-s_3-s_1} (-1)^{S-J_{13}-J_{24}} \delta_{S_{13} J_{24}} \delta_{S_{24} J_{13}} \\ &= (-1)^{S-J_{13}-s_3-s_1} \delta_{S_{13} J_{24}} \delta_{S_{24} J_{13}}. \end{aligned} \quad (8)$$

For chain lengths that are not powers of two, it turns out that a universal coupling strategy is to prime factorize the coupling scheme, i.e. the chain length. $N = 6$ for instance would be coded as $2 \cdot 3$, and so on. The recoupling coefficients contain more and more Wigner symbols as well as square roots the larger the prime factors p_i are. The maximum number of symbols per coefficient is given

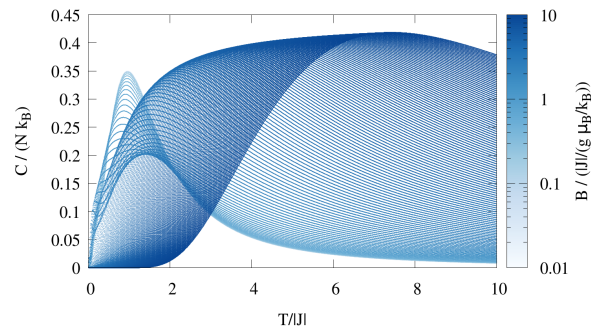
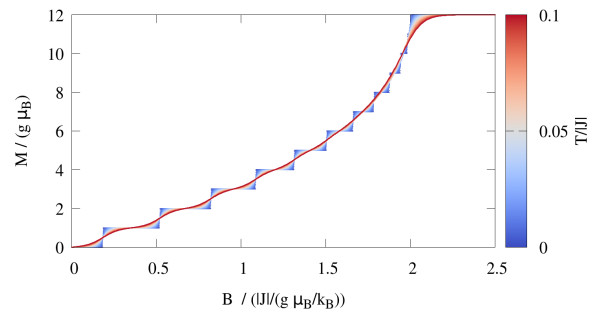
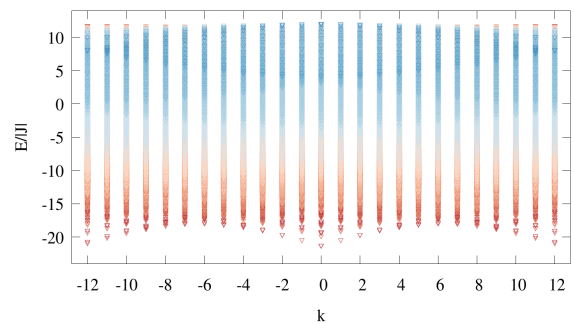
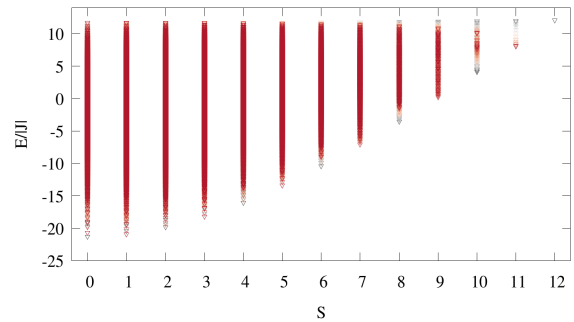


Figure 3. (Color online) Spectra and observables for an anti-ferromagnetic Heisenberg ring with $N = 24, s = 1/2$: energy spectrum vs total spin S , the same spectrum but now vs k , the magnetization vs the applied field B for various temperatures as well as the specific heat vs temperature T for various external fields (top to bottom).

by

$$N_{\text{Wigner-6J}} = \sum_{i=1}^{N_{\text{primes}}} (p_i - 2) \cdot \sum_{j=i+1}^{N_{\text{primes}}} p_j. \quad (9)$$

$N = 2^n$ fits into this scheme as the optimal case, since

only the smallest possible prime factors appear. This finding explains why a combination of spin-rotational and translational symmetry is not easily possible for the majority of system sizes – it turns into a prohibitive numerical effort to evaluate a massive number of recoupling coefficients.

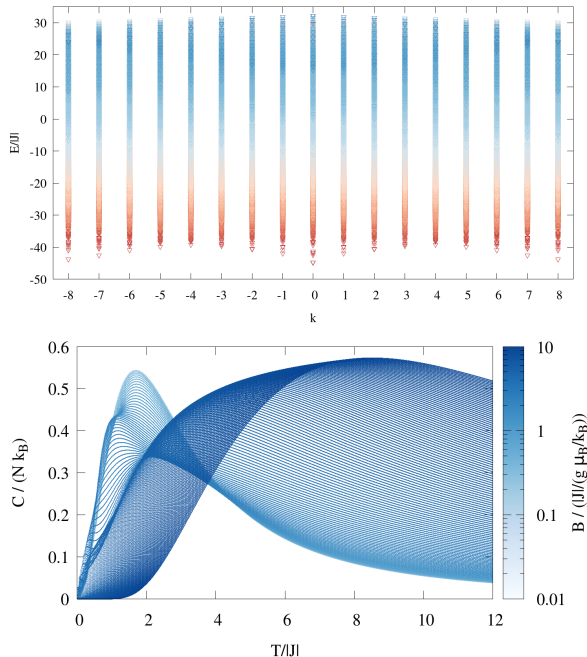


Figure 4. (Color online) Spectra and observables for an antiferromagnetic Heisenberg ring with $N = 16$, $s = 1$: energy spectrum vs k as well as the specific heat vs temperature T for various external fields (top to bottom).

III. NUMERICAL RESULTS

Finally we would like to present some of the largest cases one can actually solve nowadays. We choose Heisenberg spin rings with antiferromagnetic nearest-neighbor interaction as examples.

The first example shows spectra and magnetic observables for a spin ring with $N = 24$ sites of spins $s = 1/2$. The dimension of the total Hilbert space is $\dim(\mathcal{H}) = 16,777,216$, which can be subdivided into subspaces $\mathcal{H}(S, M = S, k)$ as outlined above. In particular, $24 = 2 * 2 * 2 * 3$. The dimension of the largest subspace $\mathcal{H}(S, M = S, k)$ is 27,275; it occurs for $S = 2$ and even $k \neq 0, 12$. Figure 3 shows from top to bottom the energy spectrum vs total spin S , the same spectrum but now vs k , the magnetization vs the applied field B for various temperatures as well as the specific heat vs temperature T for various external fields. The figures merely serve as visual proofs of the feasibility of the program than as sources for specific curves. Readers interested in the spectra or specific functions are welcome to contact the

authors.

The second example presents the results for a spin ring of $N = 16$ sites of spins $s = 1$. In this case the total dimension assumes a value of $\dim(\mathcal{H}) = 43,046,721$, which reduces to 59,143 for the largest subspace $\mathcal{H}(S, M = S, k)$ occurring for $S = 3$ and odd k . Figure 4 depicts the energy spectrum vs k as well as the specific heat vs temperature T for various external fields.

The final example of our selection deals with a fictitious spin ring of $N = 8$ spins with single-spin quantum number $s = 5$. Its main purpose is to demonstrate that the combined use of spin-rotational as well as translational symmetry allows to reduce the staggering dimension of the full Hilbert space of $\dim(\mathcal{H}) = 214,358,881$ to a rather moderate size of the largest subspace $\mathcal{H}(S, M = S, k)$ of 77,970 which occurs for $S = 9$ and odd k . Figure 5 shows the specific heat vs temperature T for various external fields calculated from all 214,358,881 levels.

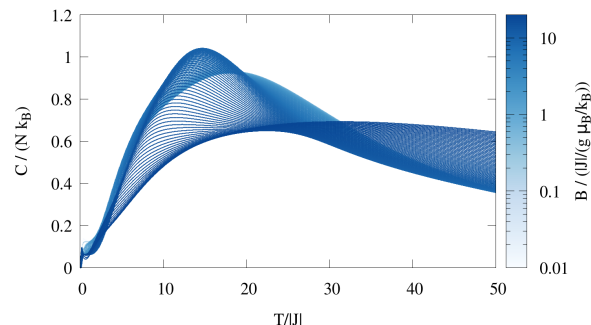


Figure 5. (Color online) Specific heat vs temperature T for various external fields for an antiferromagnetic Heisenberg ring with $N = 8$, $s = 5$.

IV. DISCUSSION AND CONCLUSIONS

The outlined method provides a valuable tool in cases where a complete and numerically exact diagonalization of a large spin system provides additional benefits compared to approximate methods. The knowledge of exact quantum numbers such as S , M , and k provides such benefits for instance in spectroscopic experiments as, for instance, inelastic neutron scattering (INS), where selection rules can be inferred.^{66–68}

The method also complements other existing exact methods, in particular Bethe ansatz methods. These work for isotropic nearest-neighbor interactions of arbitrary spin s ,^{69–73} but only for certain linear combinations of powers of $\vec{s}_i \cdot \vec{s}_{i+1}$. The most general isotropic nearest-neighbor interaction for spin s is of the form $p_s(\vec{s}_i \cdot \vec{s}_{i+1})$, where p_s denotes a polynomial of degree $2s$. For $s = 1/2$ the polynomial is simply the proportional function, which means that the Heisenberg spin-1/2 chain is integrable by Bethe ansatz. For spin-1 chains the polynomial turns out as $p_1(x) = x \pm x^2$ or $p_1(x) = x^2$, which means

that certain bilinear/biquadratic chains can be solved by Bethe ansatz.⁷⁴ Generally, the Bethe ansatz is not applicable to Heisenberg chains with only bilinear terms for $s > \frac{1}{2}$. Here (and in many other cases) our diagonalization scheme provides the exact spectra and eigenfunctions, albeit for periodic chains of restricted lengths.

Although the theoretical calculations appear straight forward, we showed that in many cases a vast number of recoupling coefficients is generated which in the worst cases yields $\dim(\mathcal{H}(S, M = S))$ coefficients for each of the $\dim(\mathcal{H}(S, M = S))/N$ states belonging to an irreducible representation (S, M, k) . This renders a practical use impossible. Nevertheless, we could also outline, for which system sizes a combined use of spin-rotational and translational symmetry is feasible. It then delivers numerically exact results for both spectra as well as observables.

Very recent numerical studies show that the range of applicability of the method can be extended, at least

somewhat, by using D_N combined with parity instead of C_N symmetry.⁷⁵ Complex valued basis coefficients and matrix elements can thereby be avoided at the cost of additional symmetry operations. This way, a complete diagonalization of a spin ring with $N = 27$ and $s = 1/2$ becomes possible, for instance.

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