PHYSICAL REVIEW B **99**, 134405 (2019)

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

Tjark Heitmann[1,*] and Jürgen Schnack[2,†]
[1]*Fachbereich für Physik, Universität Osnabrück, Barbarastrasse 7, D-49076 Osnabrück, Germany*
[2]*Fakultät für Physik, Universität Bielefeld, Postfach 100131, D-33501 Bielefeld, Germany*

(Received 7 February 2019; published 2 April 2019)

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.

DOI: 10.1103/PhysRevB.99.134405

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:

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

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 $k = 0, \dots N-1$, which 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., $[\underset{\sim}{H}, \underset{\sim}{S}^z] = 0$, one can subdivide the full Hilbert space $\mathcal{H}$ into the direct sum of all eigenspaces $\mathcal{H}(M)$ of $\underset{\sim}{S}^z$:

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

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 the density matrix renormalization group (DMRG); compare, e.g., the ALPS package [29,30].

To marry the $\underset{\sim}{S}^z$ 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 $\underset{\sim}{T}$ denotes a translation of the

---

[*] tjark.heitmann@uos.de
[†] jschnack@uni-bielefeld.de

chain by one site, i.e., the generating group operation of the translation group C_N, then

$$\begin{aligned} &|\, m_1, m_2, \dots, m_N; M, k \,\rangle \\ &\quad \propto \sum_{\nu=0}^{N-1} \big(e^{i2\pi k/N} \underset{\sim}{T}\big)^\nu \,|\, m_1, m_2, \dots, m_N; M \,\rangle \end{aligned} \tag{3}$$

is both an eigenstate of $\underset{\sim}{S}^z$ and $\underset{\sim}{T}$ 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 straightforward 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 as to 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 Sec. II we recapitulate how spin-rotational and translational symmetry can be applied simultaneously and discuss the numerical implications. Thereafter, in Sec. III we present some of the largest numerically exact calculations for spin rings, followed by a discussion in Sec. 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 $\underset{\sim}{\vec{S}}^2$ 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

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

are, e.g., generated by sequential coupling of spins along the chain. They are by construction eigenstates of $\underset{\sim}{\vec{S}}^2$ and $\underset{\sim}{S}^z$. 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 Refs. [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 nuclei [52], 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].

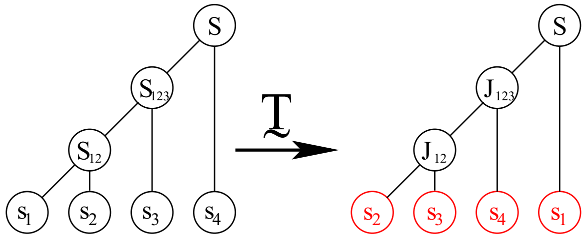

FIG. 1. Coupling schemes can be represented as coupling trees. The original sequential coupling (l.h.s.) is transformed into a sequential coupling that starts with the spin at position 2 (r.h.s.). The intermediate spins are labeled with a different letter to denote the different coupling scheme, although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

The construction of a new basis that is additionally an eigenbasis of the translation operator $\underset{\sim}{T}$ involves the projection operator already introduced in (3),

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

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 $\underset{\sim}{T}$ 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 $\underset{\sim}{T}$ 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.

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

$$\begin{aligned} \underset{\sim}{T}^\nu \,|\, \alpha, S, M \,\rangle &= \sum_{\alpha'} |\, \alpha', S, M \,\rangle \\ &\quad \times \langle\, \alpha', S, M \,|\, \underset{\sim}{T}^\nu \,|\, \alpha, S, M \,\rangle\ . \end{aligned} \tag{6}$$

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 $\langle\, \alpha', S, M = S \,|\, \underset{\sim}{T}^\nu \,|\, \alpha, S, M = S \,\rangle$. 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 possible 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

$$\begin{aligned} &|\, \alpha', S, M \,\rangle \cong |\, \alpha, S, M \,\rangle \\ \Leftrightarrow \quad &\exists \nu : \langle\, \alpha', S, M \,|\, \underset{\sim}{T}^\nu \,|\, \alpha, S, M \,\rangle \neq 0 \end{aligned} \tag{7}$$

enables us to distinguish orthogonal sets of projected states which can be orthonormalized separately. The number 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 point group used 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 the group of translations C_N also can be combined with a clever coupling scheme.

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, such as, for example, in $\langle s_1 s_2 S \mid s_2 s_1 S\rangle = (-1)^{S-s_1-s_2}$. For the example shown on the right-hand side of Fig. 2 this yields ($M = S$ omitted)

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

For chain lengths that are not powers of 2, 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 by

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

$N = 2^n$ 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.

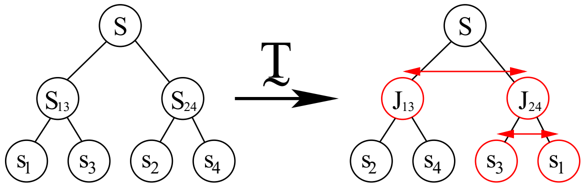

FIG. 2. Optimal coupling scheme for chain lengths of $N = 2^n$ (l.h.s.). The translated scheme (r.h.s.) can be transformed back into the old coupling scheme by spin exchange operations on the coupling graph, leading to a very simple recoupling coefficient.

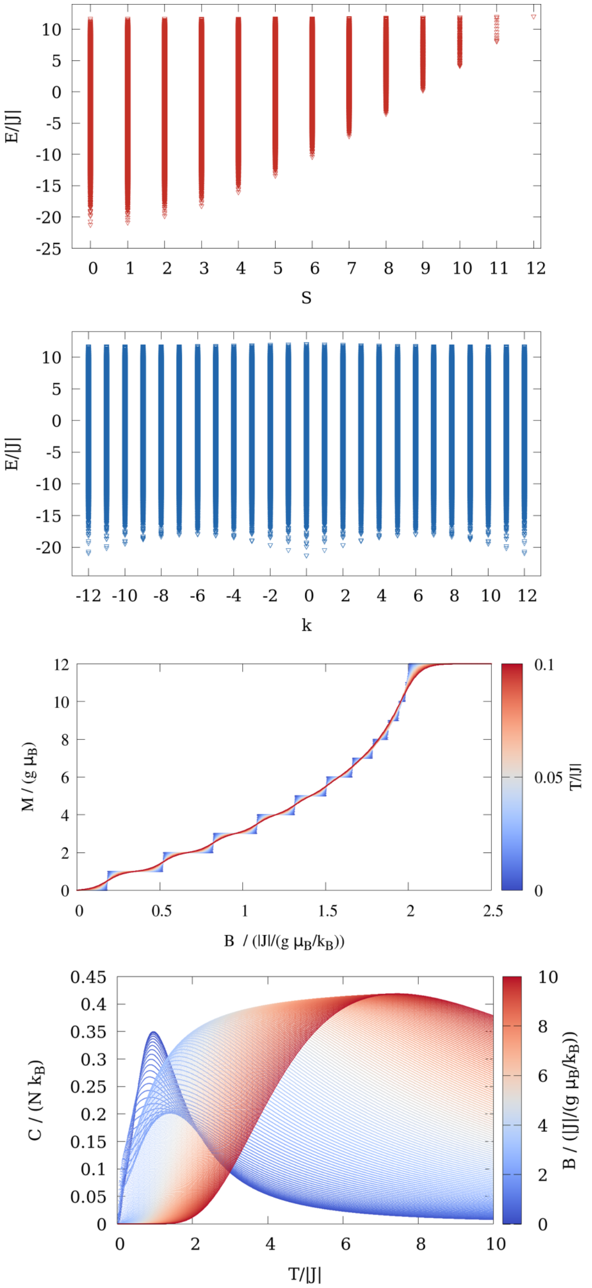

FIG. 3. Spectra and observables for an antiferromagnetic Heisenberg ring with $N = 24$, $s = 1/2$: energy spectrum vs total spin S, the same spectrum but now vs k, the magnetization vs the applied field B for various temperatures, as well as the specific heat vs temperature T for various external fields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

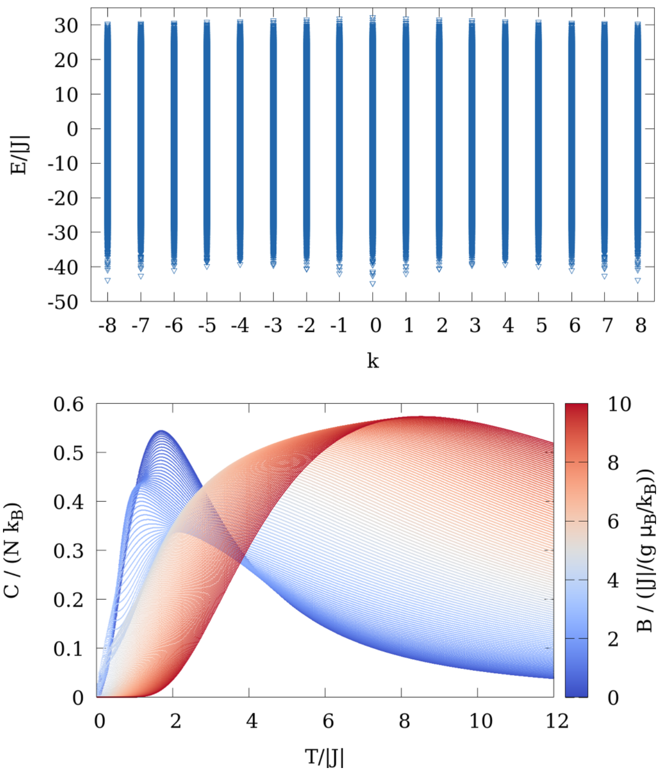

FIG. 4. Spectra and observables for an antiferromagnetic Heisenberg ring with $N = 16$, $s = 1$: energy spectrum vs k as well as the specific heat vs temperature T for various external fields (top to bottom).

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.

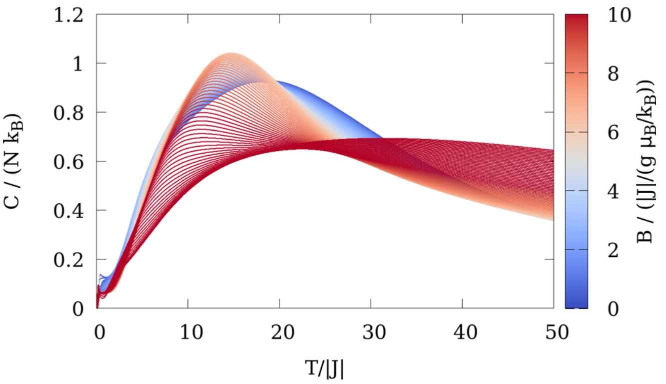

FIG. 5. Specific heat vs temperature T for various external fields for an antiferromagnetic Heisenberg ring with $N = 8$, $s = 5$.

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 one 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.

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 such 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 $\underset{\sim}{\vec{s}}_i \cdot \underset{\sim}{\vec{s}}_{i+1}$. The most general isotropic nearest-neighbor interaction for spin s is of the form $p_s(\underset{\sim}{\vec{s}}_i \cdot \underset{\sim}{\vec{s}}_{i+1})$, 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 or 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 straightforward, we showed that in many cases a vast number of recoupling coefficients are generated which in the worst cases yield $\dim(\mathcal{H}(S, M = S))$ 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.

ACKNOWLEDGMENTS

This work was supported by the Deutsche Forschungsgemeinschaft DFG [Contracts No. 314331397 (SCHN 615/23-1), No. 355031190 (FOR 2692), and No. 397300368 (SCHN 615/25-1)]. Computing time at the Leibniz Center in Garching is gratefully acknowledged. The authors thank A. Klümper and F. Göhmann for helpful discussions concerning Bethe ansatz solutions, and J. Richter as well as R. Heveling for carefully reading the manuscript.

---

[1] H. Bethe, Zur Theorie der Metalle, Z. Phys. **71**, 205 (1931).

[2] K. L. Taft, C. D. Delfs, G. C. Papaefthymiou, S. Foner, D. Gatteschi, and S. J. Lippard, $[\mathrm{Fe(OMe)_2(O_2CCH_2Cl)}]_{10}$, A molecular ferric wheel, J. Am. Chem. Soc. **116**, 823 (1994).

[3] U. Schollwöck, O. Golinelli, and T. Jolicœur, $S = 2$ antiferromagnetic quantum spin chain, Phys. Rev. B **54**, 4038 (1996).

[4] S. P. Watton, P. Fuhrmann, L. E. Pence, S. J. Lippard, A. Caneschi, A. Cornia, and G. L. Abbati, A cyclic octadecairon(III) complex, the molecular 18-wheeler, Angew. Chem. Int. Ed. **36**, 2774 (1997).

[5] T. Xiang, Thermodynamics of quantum Heisenberg spin chains, Phys. Rev. B **58**, 9142 (1998).

[6] K. Maisinger and U. Schollwöck, Thermodynamics of Frustrated Quantum Spin Chains, Phys. Rev. Lett. **81**, 445 (1998).

[7] K. Bärwinkel, H.-J. Schmidt, and J. Schnack, Structure and relevant dimension of the Heisenberg model and applications to spin rings, J. Magn. Magn. Mater. **212**, 240 (2000).

[8] O. Waldmann, Spin dynamics of finite antiferromagnetic Heisenberg spin rings, Phys. Rev. B **65**, 024424 (2001).

[9] O. Waldmann, Quantum tunneling in molecular ferric wheels, Europhys. Lett. **60**, 302 (2002).

[10] O. Waldmann, T. Guidi, S. Carretta, C. Mondelli, and A. L. Dearden, Elementary Excitations in the Cyclic Molecular Nanomagnet $\mathrm{Cr_8}$, Phys. Rev. Lett. **91**, 237202 (2003).

[11] A. V. Postnikov, J. Kortus, and S. Blügel, in *Proceedings of the Summer School on New Magnetics, Bedlewo, Poland, September 2003* [*Ab initio* simulations of Fe-based ferric wheels, Molecular Phys. Rep. **38**, 56 (2003)].

[12] M. Affronte, T. Guidi, R. Caciuffo, S. Carretta, G. Amoretti, J. Hinderer, I. Sheikin, A. G. M. Jansen, A. A. Smith, R. E. P. Winpenny, J. van Slageren, and D. Gatteschi, Mixing of magnetic states in a $\mathrm{Cr_8}$ molecular ring, Phys. Rev. B **68**, 104403 (2003).

[13] L. Engelhardt and M. Luban, Low temperature magnetization and the excitation spectrum of antiferromagnetic Heisenberg spin rings, Phys. Rev. B **73**, 054430 (2006).

[14] O. Waldmann, T. C. Stamatatos, G. Christou, H. U. Güdel, I. Sheikin, and H. Mutka, Quantum Phase Interference and Néel-Vector Tunneling in Antiferromagnetic Molecular Wheels, Phys. Rev. Lett. **102**, 157202 (2009).

[15] A. Bianchi, S. Carretta, P. Santini, G. Amoretti, T. Guidi, Y. Qiu, J. R. D. Copley, G. Timco, C. Muryn, and R. E. P. Winpenny, Rotational bands in open antiferromagnetic rings: A neutron spectroscopy study of $\mathrm{Cr_8Zn}$, Phys. Rev. B **79**, 144422 (2009).

[16] J. Dreiser, O. Waldmann, C. Dobe, G. Carver, S. T. Ochsenbein, A. Sieber, H. U. Güdel, J. van Duijn, J. Taylor, and A. Podlesnyak, Quantized antiferromagnetic spin waves in the molecular Heisenberg ring $\mathrm{CsFe_8}$, Phys. Rev. B **81**, 024408 (2010).

[17] M. L. Baker, G. A. Timco, S. Piligkos, J. S. Mathieson, H. Mutka, F. Tuna, P. Kozłowski, M. Antkowiak, T. Guidi, T. Gupta, H. Rath, R. J. Woolfson, G. Kamieniarz, R. G. Pritchard, H. Weihe, L. Cronin, G. Rajaraman, D. Collison, E. J. L. McInnes, and R. E. P. Winpenny, A classification of spin frustration in molecular magnets from a physical study of large odd-numbered-metal, odd electron rings, Proc. Natl. Acad. Sci. USA **109**, 19113 (2012).

[18] J. Ummethum, J. Nehrkorn, S. Mukherjee, N. B. Ivanov, S. Stuiber, T. Strässle, P. L. W. Tregenna-Piggott, H. Mutka, G. Christou, O. Waldmann, and J. Schnack, Discrete antiferromagnetic spin-wave excitations in the giant ferric wheel $\mathrm{Fe_{18}}$, Phys. Rev. B **86**, 104403 (2012).

[19] E. Garlatti, S. Bordignon, S. Carretta, G. Allodi, G. Amoretti, R. De Renzi, A. Lascialfari, Y. Furukawa, G. A. Timco, R. Woolfson, R. E. P. Winpenny, and P. Santini, Relaxation dynamics in the frustrated $\mathrm{Cr_9}$ antiferromagnetic ring probed by NMR, Phys. Rev. B **93**, 024424 (2016).

[20] M. Karbach, Finite-size-effekte im eindimensionalen spin-1/2-XXZ-modell, Ph.D. thesis, Bergische Universität–Gesamthochschule Wuppertal, 1994.

[21] O. Waldmann, Symmetry and energy spectrum of high-nuclearity spin clusters, Phys. Rev. B **61**, 6138 (2000).

[22] K. Bärwinkel, H.-J. Schmidt, and J. Schnack, Ground state properties of antiferromagnetic Heisenberg spin rings, J. Magn. Magn. Mater. **220**, 227 (2000).

[23] J. Schnack, Properties of the first excited state of nonbipartite Heisenberg spin rings, Phys. Rev. B **62**, 14855 (2000).

[24] K. Bärwinkel, H.-J. Schmidt, and J. Schnack, Improved upper and lower energy bounds for antiferromagnetic Heisenberg spin systems, Eur. Phys. J. B **33**, 285 (2003).

[25] W. Marshall, Antiferromagnetism, Proc. Royal. Soc. A (London) **232**, 48 (1955).

[26] E. H. Lieb, T. Schultz, and D. C. Mattis, Two soluble models of an antiferromagnetic chain, Ann. Phys. (NY) **16**, 407 (1961).

[27] E. H. Lieb and D. C. Mattis, Ordering energy levels of interacting spin systems, J. Math. Phys. **3**, 749 (1962).

[28] J. Schnack, P. Hage, and H.-J. Schmidt, Efficient implementation of the Lanczos method for magnetic systems, J. Comput. Phys. **227**, 4512 (2008).

[29] A. Albuquerque, F. Alet, P. Corboz, P. Dayal, A. Feiguin, S. Fuchs, L. Gamper, E. Gull, S. Gürtler, A. Honecker, R. Igarashi, M. Körner, A. Kozhevnikov, A. Läuchli, S. Manmana, M. Matsumoto, I. McCulloch, F. Michel, R. Noack, G. Pawłowski, L. Pollet, T. Pruschke, U. Schollwöck, S. Todo, S. Trebst, M. Troyer, P. Werner, and S. Wessel (ALPS collaboration), The

ALPS project release 1.3: Open-source software for strongly correlated systems, J. Magn. Magn. Mater. **310**, 1187 (2007).

[30] B. Bauer, L. D. Carr, H. G. Evertz, A. Feiguin, J. Freire, S. Fuchs, L. Gamper, J. Gukelberger, E. Gull, S. Guertler, A. Hehn, R. Igarashi, S. V. Isakov, D. Koop, P. N. Ma, P. Mates, H. Matsuo, O. Parcollet, G. Pawłowski, J. D. Picon, L. Pollet, E. Santos, V. W. Scarola, U. Schollwöck, C. Silva, B. Surer, S. Todo, S. Trebst, M. Troyer, M. L. Wall, P. Werner, and S. Wessel, The ALPS project release 2.0: Open source software for strongly correlated systems, J. Stat. Mech.: Theor. Exp. (2011) P05001.

[31] H. J. Schulz, T. A. L. Ziman, and D. Poilblanc, Magnetic order and disorder in the frustrated quantum Heisenberg antiferromagnet in two dimensions, J. Phys. I France **6**, 675 (1996).

[32] J. Richter, J. Schulenburg, A. Honecker, and D. Schmalfuss, Absence of magnetic order for the spin-half Heisenberg antiferromagnet on the star lattice, Phys. Rev. B **70**, 174454 (2004).

[33] I. Rousochatzakis, A. M. Läuchli, and F. Mila, Highly frustrated magnetic clusters: The kagomé on a sphere, Phys. Rev. B **77**, 094420 (2008).

[34] J. Richter and J. Schulenburg, The spin-1/2 J_1-J_2 Heisenberg antiferromagnet on the square lattice: Exact diagonalization for $N = 40$ spins, Eur. Phys. J. B **73**, 117 (2010).

[35] J. Schulenburg, SPINPACK 2.56 (Otto von Guericke University Magdeburg, Magdeburg, Germany, 2017).

[36] V. Zauner-Stauber, L. Vanderstraeten, J. Haegeman, I. P. McCulloch, and F. Verstraete, Topological nature of spinons and holons: Elementary excitations from matrix product states with conserved symmetries, Phys. Rev. B **97**, 235155 (2018).

[37] D. Gatteschi and L. Pardi, Magnetic-properties of high-nuclearity spin clusters—A fast and efficient procedure for the calculation of the energy-levels, Gazz. Chim. Ital. **123**, 231 (1993).

[38] J. J. Borras-Almenar, J. M. Clemente-Juan, E. Coronado, and B. S. Tsukerblat, High-nuclearity magnetic clusters: Generalized spin Hamiltonian and its use for the calculation of the energy levels, bulk magnetic properties, and inelastic neutron scattering spectra, Inorg. Chem. **38**, 6081 (1999).

[39] A. Bencini and D. Gatteschi, *Electron Paramagnetic Resonance of Exchange Coupled Systems* (Springer, Berlin, 1990).

[40] B. S. Tsukerblat, *Group Theory in Chemistry and Spectroscopy: A Simple Guide to Advanced Usage*, 2nd ed. (Dover Publications, Mineola, New York, 2006).

[41] B. Tsukerblat, Group-theoretical approaches in molecular magnetism: Metal clusters, Inorg. Chim. Acta **361**, 3746 (2008).

[42] A. S. Boyarchenkov, I. G. Bostrem, and A. S. Ovchinnikov, Quantum magnetization plateau and sign change of the magnetocaloric effect in a ferrimagnetic spin chain,Phys. Rev. B **76**, 224410 (2007).

[43] R. Schnalle and J. Schnack, Numerically exact and approximate determination of energy eigenvalues for antiferromagnetic molecules using irreducible tensor operators and general point-group symmetries, Phys. Rev. B **79**, 104419 (2009).

[44] R. Schnalle and J. Schnack, Calculating the energy spectra of magnetic molecules: Application of real- and spin-space symmetries, Int. Rev. Phys. Chem. **29**, 403 (2010).

[45] J. J. Borras-Almenar, J. M. Clemente-Juan, E. Coronado, and B. S. Tsukerblat, MAGPACK1—A package to calculate the energy levels, bulk magnetic properties, and inelastic neutron scattering spectra of high nuclearity spin clusters, J. Comp. Chem. **22**, 985 (2001).

[46] I. P. McCulloch and M. Gulacsi, The non-Abelian density matrix renormalization group algorithm, Europhys. Lett. **57**, 852 (2002).

[47] I. P. McCulloch, From density-matrix renormalization group to matrix product states, J. Stat. Mech.: Theory Exp. (2007) P10014.

[48] A. Fledderjohann, A. Klümper, and K.-H. Mütter, Diagrammatics for SU(2) invariant matrix product states, J. Phys. A: Math. Theor. **44**, 475302 (2011).

[49] G. Alvarez, Implementation of the SU(2) Hamiltonian symmetry for the DMRG algorithm, Comp. Phys. Commun. **183**, 2226 (2012).

[50] A. Weichselbaum, Non-Abelian symmetries in tensor networks: A quantum symmetry space approach, Ann. Phys. **327**, 2972 (2012).

[51] R. Zadourian, A. Fledderjohann, and A. Klümper, Matrix product states for SU(2) invariant quantum spin chains, J. Stat. Mech.: Theor. Exp. (2016) 083101.

[52] J. Dukelsky and S. Pittel, The density matrix renormalization group for finite fermi systems, Rep. Prog. Phys. **67**, 513 (2004).

[53] I. Affleck, Z. Zou, T. Hsu, and P. W. Anderson, SU(2) gauge symmetry of the large-U limit of the Hubbard model, Phys. Rev. B **38**, 745 (1988).

[54] S. Zhang, SO(4) symmetry of the Hubbard model and its experimental consequences, Int. J. Mod. Phys. B **5**, 153 (1991).

[55] P. A. Lee, N. Nagaosa, T.-K. Ng, and X.-G. Wen, SU(2) formulation of the $t - J$ model: Application to underdoped cuprates, Phys. Rev. B **57**, 6003 (1998).

[56] R. Schumann, Thermodynamics of a 4-site Hubbard model by analytical diagonalization, Ann. Phys.-Berlin **11**, 49 (2002).

[57] R. Thomale, S. Rachel, P. Schmitteckert, and M. Greiter, Family of spin-S chain representations of SU$(2)_k$ Wess-Zumino-Witten models, Phys. Rev. B **85**, 195149 (2012).

[58] P. Nataf and F. Mila, Exact Diagonalization of Heisenberg SU(N) Models, Phys. Rev. Lett. **113**, 127204 (2014).

[59] P. Nataf and F. Mila, Exact diagonalization of Heisenberg SU(N) chains in the fully symmetric and antisymmetric representations, Phys. Rev. B **93**, 155134 (2016).

[60] K. Wan, P. Nataf, and F. Mila, Exact diagonalization of SU(N) Heisenberg and Affleck-Kennedy-Lieb-Tasaki chains using the full SU(N) symmetry, Phys. Rev. B **96**, 115159 (2017).

[61] V. Fack, S. N. Pitre, and J. van der Jeugt, New efficient programs to calculate general recoupling coefficients, Part II: Evaluation of a summation formula, Comp. Phys. Comm. **86**, 105 (1995).

[62] V. Fack, S. N. Pitre, and J. van der Jeugt, Calculation of a general recoupling coefficient using graphical methods, Comp. Phys. Comm. **101**, 155 (1997).

[63] C. Delfs, D. Gatteschi, L. Pardi, R. Sessoli, K. Wieghardt, and D. Hanke, Magnetic properties of an octanuclear iron(III) cation, Inorg. Chem. **32**, 3099 (1993).

[64] I. G. Bostrem, A. S. Ovchinnikov, and V. E. Sinitsyn, The method of exact diagonalization preserving the total spin and taking the point symmetry of the two-dimensional isotropic Heisenberg magnet into account, Theor. Math. Phys. **149**, 1527 (2006).

[65] V. E. Sinitsyn, I. G. Bostrem, and A. S. Ovchinnikov, Symmetry adapted finite-cluster solver for quantum Heisenberg model in two dimensions: A real-space renormalization approach, J. Phys. A-Math. Theor. **40**, 645 (2007).

[66] A. Furrer, Magnetic cluster excitations, Int. J. Mod. Phys. B **24**, 3653 (2010).

[67] M. L. Baker, T. Guidi, S. Carretta, J. Ollivier, H. Mutka, H. U. Güdel, G. A. Timco, E. J. L. McInnes, G. Amoretti, R. E. P. Winpenny, and P. Santini, Spin dynamics of molecular nanomagnets unravelled at atomic scale by four-dimensional inelastic neutron scattering, Nat. Phys. **8**, 906 (2012).

[68] A. Furrer and O. Waldmann, Magnetic cluster excitations, Rev. Mod. Phys. **85**, 367 (2013).

[69] P. P. Kulish, N. Yu. Reshetikhin, and E. K. Sklyanin, Yang-Baxter equation and representation theory: I, Lett. Math. Phys. **5**, 393 (1981).

[70] L. Takhtajan, The picture of low-lying excitations in the isotropic Heisenberg chain of arbitrary spins, Phys. Lett. A **87**, 479 (1982).

[71] H. Babujian, Exact solution of the isotropic Heisenberg chain with arbitrary spins: Thermodynamics of the model, Nucl. Phys. B **215**, 317 (1983).

[72] A. Tsvelick, The exact solution of 2D ZN invariant statistical models, Nucl. Phys. B **305**, 675 (1988).

[73] H. Frahm, N.-C. Yu, and M. Fowler, The integrable XXZ Heisenberg model with arbitrary spin: Construction of the Hamiltonian, the ground-state configuration, and conformal properties, Nucl. Phys. B **336**, 396 (1990).

[74] S. R. Manmana, A. M. Läuchli, F. H. L. Essler, and F. Mila, Phase diagram and continuous pair-unbinding transition of the bilinear-biquadratic $S = 1$ Heisenberg chain in a magnetic field, Phys. Rev. B **83**, 184433 (2011).

[75] A. W. Sandvik, in *Lectures on the Physics of Strongly Correlated Systems XIV: Fourteenth Training Course in the Physics of Strongly Correlated Systems*, edited by A. Avella and F. Mancini, AIP Conf. Proc. No. 1297 (AIP, New York, 2010), p. 135.