Exact Diagonalization of Heisenberg SU(N) Models

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(Received 23 May 2014; published 18 September 2014)

Building on advanced results on permutations, we show that it is possible to construct, for each irreducible representation of SU(N), an orthonormal basis labeled by the set of *standard Young tableaux* in which the matrix of the Heisenberg SU(N) model (the quantum permutation of N-color objects) takes an explicit and extremely simple form. Since the relative dimension of the full Hilbert space to that of the singlet space on n sites increases very fast with N, this formulation allows us to extend exact diagonalizations of finite clusters to much larger values of N than accessible so far. Using this method, we show that, on the square lattice, there is long-range color order for SU(5), spontaneous dimerization for SU(8), and evidence in favor of a quantum liquid for SU(10).

DOI: 10.1103/PhysRevLett.113.127204 PACS numbers: 75.10.Jm, 02.70.-c, 67.85.-d, 71.10.Fd

There is currently considerable experimental activity on ultracold multicomponent fermions [1–3]. When loaded in an optical lattice, these systems are expected to be, for integer number of particles per site and sufficiently large on-site repulsion, in a Mott insulating phase described by the SU(N) Heisenberg model [4–7]. This effective model is a generalization of the familiar SU(2) model, and in the case of one particle per site, it takes the general form of a quantum permutation Hamiltonian:

$$H = \sum_{(i,j)} J_{ij} \sum_{\mu,\gamma=A,B,C,\ldots} |\mu_i \gamma_j\rangle\langle\gamma_i \mu_j| = \sum_{(i,j)} J_{ij} P_{ij}, \qquad (1)$$

where the sum $\sum_{(i,j)}$ runs over all pairs of interacting sites (J_{ij} being the coupling constant). The *permutation* operator P_{ij} simply switches the states between sites i and j, and the local Hilbert space is of dimension N.

In the context of condensed matter physics, two cases have been mainly studied: SU(3), which describes spins 1 with a biquadratic interaction equal to the bilinear one [8–10], and SU(4), the symmetric version of the Kugel-Khomskii spin-orbital model [11–14]. Apart from one dimension, where there is a Bethe ansatz solution [15] and minus sign free quantum Monte Carlo simulations [16,17], reliable information could only be obtained by combining approximate analytical and numerical approaches such as flavor-wave theory [8,18], exact diagonalizations (EDs) of finite clusters [9,19–21], variational Monte Carlo [20–22], or tensor network algorithms [19,20,23].

With cold atoms, one can implement larger values of N, up to 10, allowing one to realize new types of quantum phases [7]. In particular, it has been predicted by mean-field theory that chiral phases might be stabilized for large enough N [24–26]. However, for large N, most of the methods employed encounter specific difficulties: flavor-wave theory is limited to phases with long-range color order, the performance of tensor-network algorithms significantly decreases when the dimension of the local Hilbert space increases, and EDs are severely limited by the size of the available clusters. Alternatives are clearly called for.

In this Letter, we introduce a simple method to perform EDs of any quantum permutation Hamiltonian separately in each irreducible representation (irrep) of SU(N). Since the dimension of the irreps relevant at low energy (for instance the singlet, to which the ground state belongs) is much smaller than that of the sector used in traditional ED, this approach allows one to perform ED on essentially the same cluster sizes for large N as for small N. The power of the method is illustrated by the first and only ED investigation so far of SU(5), SU(8), and SU(10) on the square lattice.

Let us first recall some standard results about the irreps of SU(N). For a lattice of n sites, each irrep can be associated to a Young tableau with n boxes and at most N rows (see Fig. 1). The shape of a Young tableau can be described by an array $\alpha = [\alpha_1, \alpha_2, \ldots, \alpha_k]$ $(1 \le k \le N)$ where the lengths of the rows α_j satisfy $\alpha_1 \ge \alpha_2 \ge \ldots \ge \alpha_k \ge 1$. In the full Hilbert space $\square^{\otimes n}$, where $\square$ is the fundamental irrep or equivalently the Hilbert space for one site, the multiplicity f^α of an irrep, i.e., the number of times it appears, is given by $f^\alpha = n!/(\prod_{i=1}^n l_i)$, where the hook length l_i of a box is defined as the number of boxes on the same row at the right plus the number of boxes in the same column below plus the box itself (see Fig. 1). The multiplicity is equal to the number of standard Young tableaux, i.e., Young tableaux filled up with numbers from 1 to n in ascending order from left to right in any row, and from top to bottom in any column. The standard Young tableaux can be ranked from 1 to f^α through the last letter sequence: two standard tableaux S_r and S_s are such that $S_r < S_s$ if the number n appears in S_r in a row below the one in which it appears in S_s. If those rows are the same, one looks at the rows of $n-1$, etc. (see Fig. 1). The dimension d_N^α of an irrep can also be calculated very simply from the shape α as $d_N^\alpha = \prod_{i=1}^n (d_{i,N}/l_i)$, where $d_{i,N} = N + \gamma_i$, where γ_i is the

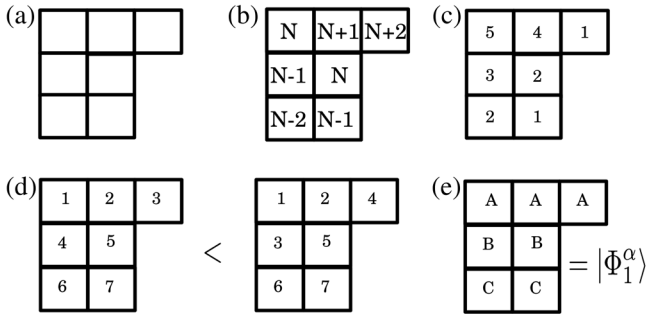
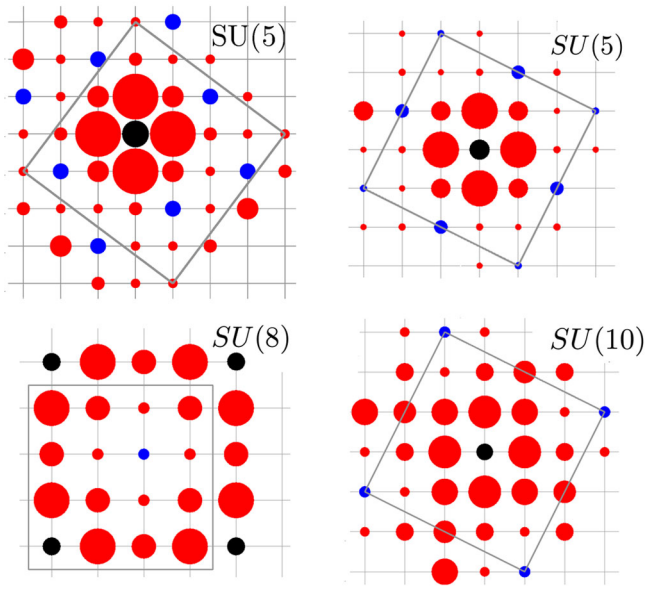


FIG. 1. (a) Example of a Young tableau: $\alpha = [3,2,2]$; (b) Integers $d_{i,N}$ that enter the numerator of the dimension of α; (c) Hook lengths l_i; (d) Examples of standard tableaux ranked according to the *last letter sequence*. (e) Normal product state $|\Phi_1^{[3,2,2]}\rangle = |AAABBCC\rangle$.

algebraic distance from the ith box to the main diagonal, counted positively (resp. negatively) for a box above (below) the diagonal (see Fig. 1). The full Hilbert space can be decomposed as $\square^{\otimes n} = \oplus_\alpha V^\alpha$, where V^α is the Hilbert space associated to irrep α, and, if $d_N^\alpha > 1$, V^α can itself be decomposed into d_N^α equivalent subsectors V_i^α as $V^\alpha = \oplus_i V_i^\alpha$, with $\dim(V_i^\alpha) = f^\alpha$, $\dim(V^\alpha) = f^\alpha d_N^\alpha$ and $\dim(\square^{\otimes n}) = N^n = \sum_\alpha f^\alpha d_N^\alpha$ [27].

For our purpose, the key property is that, since it has SU(N) symmetry, the quantum permutation Hamiltonian H can be diagonalized independently in each subsector V_i^α, whose size (in particular that of the singlet) becomes much smaller than that of the Hilbert space used in standard ED when N increases (see examples in the table of Fig. 2 and Supplemental Material [28]). To diagonalize H directly in a subsector V_i^α, one should construct an orthonormal basis of this sector, and write the matrix of H in this basis. In principle, one can construct a basis recursively using SU(N) Clebsch-Gordan coefficients [30]. However, since the multiplicity of an irrep is equal to the number of standard Young tableaux, a natural alternative is to try and associate directly a basis state to each standard Young tableau. This can be achieved by using the Young symmetrization operator, the product of antisymmetrizers on the columns followed by symmetrizers on the rows [31]. Indeed, one can get a set of f^α linearly independent states that all belong to irrep α by applying the Young symmetrization operator associated with a standard tableau S_r, in which the sites involved in the symmetrizers and antisymmetrizers are chosen according to the numbering of S_r, to the product state: $|\Phi_r^\alpha\rangle = |\sigma_1\rangle \otimes \ldots \otimes |\sigma_n\rangle$, with $|\sigma_i\rangle = A$ if i belongs to the first line of S_r, B if it belongs to its second line, etc. [28]. However, this construction does not lead to a simple method to perform ED of the SU(N) Heisenberg model for two reasons. First, these states are not orthogonal. Besides, the Hamiltonian does not take a simple form.

In his substitutional analysis, Young also realized that the Young symmetrization operators (called *natural units* in his original work [32]) were not convenient to solve algebraic problems [33]. So, he further developed the theory of the permutation group to come up with more powerful operators than the simple products of symmetrizers and antisymmetrizers. More specifically, he constructed linear superpositions of permutations of the symmetric group $\mathcal{S}_n$ that he called *orthogonal units* which, when interpreted as operators in the Hilbert space of the SU(N) Heisenberg model, will enable us to construct an orthonormal basis in which the quantum permutation Hamiltonian takes a very simple form. For a fixed shape α, there are $(f^\alpha)^2$ orthogonal units $\{o_{rs}^\alpha\}_{r,s=1..f^\alpha}$, where the indices r and s refer to two standard tableaux of shape α. They can be constructed recursively as nested products of symmetrizers and antisymmetrizers associated to standard tableaux of smaller size [28,34]. The resulting expressions are rather complicated. For instance, for the shape $[2,1]$ ($n = 3$), for which there are two standard tableaux, the first orthogonal unit reads $o_{11}^{[2,1]} = (1/12)(\epsilon + \tau_{1,2})^2(\epsilon - \tau_{1,3})(\epsilon + \tau_{1,2})$ where



$SU(N)$	n	$f^{[k,\ldots,k]}$	$\frac{(n-1)!}{k!^N}$	$\mathcal{E}_{GS}$
$SU(5)$	25 (tilted)	701149020	2.5×10^{13}	-1.154324
$SU(5)$	25 (5×5)	701149020	2.5×10^{13}	-1.164712
$SU(5)$	20	1662804	1.5×10^{10}	-1.215377
$SU(8)$	16	1430	5.1×10^{9}	-1.572223
$SU(10)$	20	16796	1.2×10^{14}	-1.589218

FIG. 2 (color online). Real-space correlations $\langle P_{0j}\rangle - 1/N$ for various SU(N) models and cluster sizes on the square lattice with periodic boundary conditions: SU(5) (tilted 25 and 20 site cluster), SU(8) (16 sites), and SU(10) (20 sites). The black dot is the reference site 0. Positive (negative) correlations are depicted as blue (red) disks with an area proportional to the absolute value of the correlation. The correlations for SU(5) on the (5×5) 25-site cluster are shown and discussed in the Supplemental Material [28]. Table: dimension $f^{[n/N,\ldots,n/N]}$ of the singlet subspace in which the permutation Hamiltonian has been diagonalized, approximate dimension $(n-1)!/(n/N)!^N$ of the Hilbert space used in standard ED [29], ground states energies per site $\mathcal{E}_{\mathrm{GS}}$.

$\tau_{i,j}$ denotes the transposition $i \leftrightarrow j$ and ϵ is the identity for $\mathcal{S}_n$. In practice however, we will never need the explicit expressions of the orthogonal units, but only some of their properties derived by Young that we now summarize.

(i) They satisfy orthonormal relations: $\forall \alpha, \beta$

$$o^{\alpha}_{rs} o^{\beta}_{uv} = \delta^{\alpha\beta} \delta_{su} o^{\alpha}_{rv} \quad \forall\ r,s = 1 \ldots f^{\alpha}, \quad \forall\ u,v = 1 \ldots f^{\beta}. \tag{2}$$

(ii) The projector onto the irrep α can be decomposed as $T^{\alpha} = \sum_{r=1\ldots f^{\alpha}} o^{\alpha}_{rr}$.

(iii) They provide a basis in which every linear superposition of permutations of $\mathcal{S}_n$ can be uniquely decomposed, a simple consequence of Eq. (2) and of the identity $\sum_{\alpha} f^2_{\alpha} = n!$ [32]. In particular, the Hamiltonian of Eq. (1) can be written as $H = \sum_{\beta,t,q} \mu^{\beta}_{tq}(H) o^{\beta}_{tq}$, where $\mu^{\beta}_{tq}(H)$ are real coefficients.

(iv) The decomposition of *successive transpositions*, i.e., transpositions between consecutive numbers $\tau_{k,k+1}$ $(1 \le k \le n-1)$, takes a very simple form. In fact, if we write $\tau_{k,k+1} = \sum_{\beta,t,q} \mu^{\beta}_{tq}(\tau_{k,k+1}) o^{\beta}_{tq}$, then, for a given shape α, the matrices $\bar{\bar{\mu}}^{\alpha}(\tau_{k,k+1})$ defined by $[\bar{\bar{\mu}}^{\alpha}(\tau_{k,k+1})]_{tu} = \mu^{\alpha}_{tu}(\tau_{k,k+1})$ are orthogonal and very sparse, with at most two nonvanishing entries per column or per line that can be calculated easily. More precisely, if $k+1$ and k are in the same row (resp. column) in S_t, then $\mu^{\alpha}_{tt}(\tau_{k,k+1}) = +1$ (resp. -1), and all other matrix elements involving t vanish. If $k+1$ and k are not in the same column or the same line, and if S_u is the tableau obtained from S_t by interchanging k and $k+1$, then the only nonvanishing matrix elements involving t or u are given by

$$\begin{pmatrix} \mu^{\alpha}_{tt}(\tau_{k,k+1}) & \mu^{\alpha}_{tu}(\tau_{k,k+1}) \\ \mu^{\alpha}_{ut}(\tau_{k,k+1}) & \mu^{\alpha}_{uu}(\tau_{k,k+1}) \end{pmatrix} = \begin{pmatrix} -\rho & \sqrt{1-\rho^2} \\ \sqrt{1-\rho^2} & \rho \end{pmatrix},$$

where ρ is the inverse of *the axial distance* from k to $k+1$ in S_t defined by counting $+1$ (resp. -1) for each step made downwards or to the left (resp. upwards or to the right) to reach $k+1$ from k. For instance, $\tau_{3,4}$ has nonvanishing matrix elements between the two tableaux of Fig. 1(d), with diagonal matrix elements equal to $-1/3$ (left tableau) and $1/3$ (right tableau), and off-diagonal matrix elements equal to $2\sqrt{2}/3$.

(v) The matrix $\bar{\bar{\mu}}^{\beta}(\sigma)$ that enters the decomposition of any permutation $\sigma = \sum_{\beta,t,q} \mu^{\beta}_{tq}(\sigma) o^{\beta}_{tq}$ is also orthogonal. Indeed, a permutation can be decomposed as a product of transpositions, and any transposition $\tau_{i,j}$ can be decomposed as a product of successive transpositions according to (assuming $i < j$)

$$\tau_{i,j} = \tau_{i,i+1}\tau_{i+1,i+2} \ldots \tau_{j-1,j}\tau_{j-2,j-1} \ldots \tau_{i+1,i+2}\tau_{i,i+1},$$

so that the matrix $\bar{\bar{\mu}}^{\beta}(\sigma)$ is a product of orthogonal matrices.

To prove the central results of this Letter, we need an additional property not derived by Young:

Lemma: When interpreted as operators acting in the Hilbert space, the orthogonal units satisfy

$$(o^{\beta}_{rs})^{\dagger} = o^{\beta}_{sr}. \tag{3}$$

Proof:—The decomposition of the permutations can be inverted as $o^{\beta}_{rs} = (f^{\beta}/n!) \sum_{\sigma \in \mathcal{S}_n} \mu^{\beta}_{sr}(\sigma^{-1}) \sigma$ [32,33]. Now, $\bar{\bar{\mu}}^{\beta}(\sigma^{-1}) = [\bar{\bar{\mu}}^{\beta}(\sigma)]^{-1}$, and since $\bar{\bar{\mu}}^{\beta}(\sigma)$ is orthogonal, $[\bar{\bar{\mu}}^{\beta}(\sigma)]^{-1}_{sr} = [\bar{\bar{\mu}}^{\beta}(\sigma)]_{rs}$, so that $\mu^{\beta}_{sr}(\sigma^{-1}) = \mu^{\beta}_{rs}(\sigma)$. Then, since the adjoint operator of any permutation σ is $\sigma^{\dagger} = \sigma^{-1}$, we can write

$$(o^{\beta}_{rs})^{\dagger} = \frac{f^{\beta}}{n!} \sum_{\sigma \in S_n} \mu^{\beta}_{sr}(\sigma^{-1}) \sigma^{\dagger} = \frac{f^{\beta}}{n!} \sum_{\sigma \in S_n} \mu^{\beta}_{rs}(\sigma) \sigma^{-1} = o^{\beta}_{sr}.$$

We are now in a position to state and demonstrate the two central results of this Letter.

Proposition 1: Let $|\Phi^{\alpha}_1\rangle$ be the product state associated to the first standard tableau S_1 [see Fig. 1(e)]. Then, the set

$$\{|\Psi^{\alpha}_r\rangle = ||o^{\alpha}_{11}|\Phi^{\alpha}_1\rangle||^{-1} o^{\alpha}_{r1}|\Phi^{\alpha}_1\rangle\}_{r=1\ldots f^{\alpha}}$$

is an orthonomal basis of one of the subsectors of V^{α}.

Proof:—$\langle \Psi^{\alpha}_l | \Psi^{\alpha}_r \rangle = ||o^{\alpha}_{11}|\Phi^{\alpha}_1\rangle||^{-2} \langle \Phi^{\alpha}_1 | (o^{\alpha}_{l1})^{\dagger} o^{\alpha}_{r1} | \Phi^{\alpha}_1 \rangle = ||o^{\alpha}_{11}|\Phi^{\alpha}_1\rangle||^{-2} \langle \Phi^{\alpha}_1 | o^{\alpha}_{1l} o^{\alpha}_{r1} | \Phi^{\alpha}_1 \rangle = \delta_{lr}$, where we have used that $o^{\alpha}_{11}|\Phi^{\alpha}_1\rangle \neq 0$ [28]. Besides, the states transform according to the irrep α since $o^{\alpha}_{r1}|\Phi^{\alpha}_1\rangle = o^{\alpha}_{rr} o^{\alpha}_{r1}|\Phi^{\alpha}_1\rangle = T^{\alpha} o^{\alpha}_{r1}|\Phi^{\alpha}_1\rangle \in V^{\alpha}$. Finally, from Eq. (2), the set is obviously invariant under any permutation. So it must generate a subsector of V^{α}.

Proposition 2: The matrix elements of H in this basis are

$$\langle \Psi^{\alpha}_r | H | \Psi^{\alpha}_s \rangle = \mu^{\alpha}_{rs}(H). \tag{4}$$

Proof:—This is a simple consequence of Eq. (2).

These coefficients are simply related to those of transpositions by $\mu^{\beta}_{rs}(H) = \sum_{(i,j)} J_{ij} \mu^{\beta}_{rs}(\tau_{i,j})$, which are themselves products of the sparse matrices of successive transpositions whose explicit form has been given in point (iv) above. So, we have succeeded in constructing an orthonormal basis of one subsector of any irrep, and we have come up with a very simple scheme to construct the matrix of the Hamiltonian in this basis. Let us emphasize that the explicit calculation of the basis is *not* required to calculate the matrix elements of the Hamiltonian or of any operator that can be written as a permutation.

We have used this theory to numerically investigate the antiferromagnetic Heisenberg SU(N) Hamiltonian on the square lattice [Eq. (1) with $J_{ij} = J$ for pairs of nearest neighbors and 0 otherwise] for $N = 5$ (20 and 25 sites), $N = 8$ (16 sites), and $N = 10$ (20 sites). In each case, we have calculated the real-space correlations $\langle P_{0j} \rangle - 1/N$, the

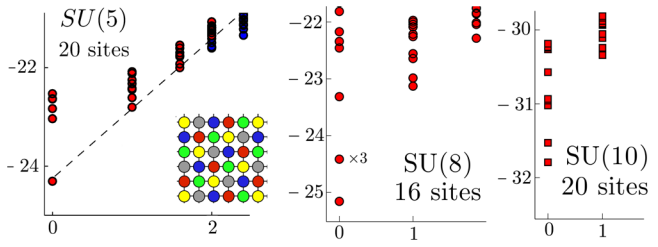


FIG. 3 (color online). Energy spectra (in units of J) for SU(5) (20 sites), SU(8) (16 sites), and SU(10) (20 sites), plotted as a function of the quadratic Casimir operator C_2 (See Refs. [28,38]). Different irreps with the same C_2 [e.g., $C_2 = 2$ for SU(5)] are represented with different colors. Below the SU(5) tower of states, sketch of the long-ranged color ordered pattern consistent with the real-space correlations of Fig. 2 and with flavor-wave theory.

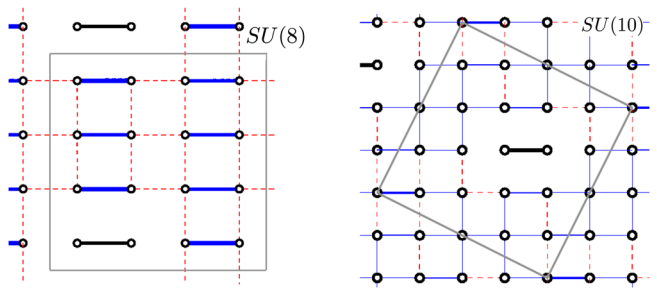


FIG. 4 (color online). Dimer-dimer correlations $\langle P_{ij}P_{\mathrm{ref}}\rangle - \langle P_{\mathrm{ref}}\rangle^2$ for SU(8) (16 sites) and SU(10) (20 sites). The reference bond is shown in black while positive (negative) correlations are shown as solid blue (dashed red) lines, with a thickness proportional to the dimer-dimer correlation.

low energy spectrum, and the dimer-dimer correlations $\langle P_{ij}P_{\mathrm{ref}}\rangle - \langle P_{\mathrm{ref}}\rangle^2$. Some basic information (size of Hilbert space, ground state energy) is summarized in the table of Fig. 2.

As can be seen in Fig. 2, short-range color order is clearly present in all cases, with positive correlations which point to an N-site periodicity. To check whether these correlations are actually long ranged, the best way with ED is to look at the low-energy spectrum, which is expected to build an Anderson tower of states [35–37] if the SU(N) symmetry is broken in the ground state [9]. As can be seen from Fig. 3, this is clearly the case for SU(5). We have actually been able to calculate the full low-energy spectrum for $N = 5$ on 20 sites, whose structure illustrates several general features of SU(N) models [28]. The ordering pattern suggested by real-space correlations is consistent with linear flavor-wave theory which predicts that, up to a mirror reflection (and of course to color permutation), there is a single pattern (shown as an inset of the SU(5) tower of states in Fig. 3) able to minimize the zero point energy on each bond [28].

For SU(8), the spectrum has a very different structure: there is a threefold degenerate singlet far below the first nonsinglet excited states, as in the case of SU(4), and with the same quantum numbers [14,19]. This is typical of a translational symmetry breaking, and the quantum numbers [two states of zero momentum, one state of momentum $(\pi, 0)$ and one state of momentum $(0, \pi)$] are compatible with a spontaneous dimerization with columns or rows of dimers. This possibility is clearly confirmed by the dimer-dimer correlations of Fig. 4, which point to well-developed long-range dimer order. These correlations are very similar to those of SU(4), in which case infinite projected entangled pair states simulations have been able to further confirm the nature of the instability [19]. So EDs clearly point to spontaneous dimerization for SU(8). Of course, since it takes eight (or a multiple of eight) sites to build a singlet for SU(8), the dimers are not singlets, but they build an irrep of dimension $N(N-1)/2 = 28$. Whether these effective degrees of freedom develop some kind of order cannot be decided on the basis of the present results.

Finally, the case of SU(10) is again quite different. In that case, dimer-dimer correlations do not point to any kind of dimer order, and there are several low-lying singlets below the first nonsinglet excitation. This is reminiscent of the situation observed in SU(2) quantum spin liquids, such as the kagome antiferromagnet [39–41], with which the present model shares another remarkable property, a massive classical degeneracy [42]. So the most likely possibility is that this system is a quantum spin liquid.

To summarize, we have introduced a simple and explicit formulation of the quantum permutation Hamiltonian separately in each irreducible representation of SU(N). We have illustrated the power of the method on a problem of considerable current interest, the properties of ultracold multicomponent fermionic atoms loaded in an optical lattice, opening the way to the investigation of much larger values of N than accessible so far. This approach is also expected to be very powerful on other problems. For instance, it should be competitive even for smaller values of N in the presence of disorder since there is no spatial symmetry to reduce the size of the Hilbert space of standard exact diagonalizations. The method can also be extended to the general case of the SU(N) Heisenberg model with any irrep at each site, a model relevant, e.g., to Mott phases with more than one fermion per site for which chiral phases have been predicted [24,25]. The very simple structure of the basis and of the Hamiltonian should also lead to alternative formulations of other numerical simulations, in particular, density matrix renormalization group simulations. Work is in progress along these lines.

The authors acknowledge P. Corboz, M. Hermele, A. Läuchli, K. Penc, N. Schellekens, and J-B. Zuber for useful discussions. This work has been supported by the Swiss National Fund.

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