Variational Monte-Carlo investigation of SU(N) Heisenberg chains

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Motivated by recent experimental progress in the context of ultra-cold multi-color fermionic atoms in optical lattices, we have investigated the properties of the SU(N) Heisenberg chain with totally antisymmetric irreducible representations, the effective model of Mott phases with $m < N$ particles per site. These models have been studied for arbitrary $N$ and $m$ with non-abelian bosonization [I. Affleck, Nuclear Physics B 265, 409 (1986); 305, 582 (1988)], leading to predictions about the nature of the ground state (gapped or critical) in most but not all cases. Using exact diagonalization and variational Monte-Carlo based on Gutzwiller projected fermionic wave functions, we have been able to verify these predictions for a representative number of cases with $N \leq 10$ and $m \leq N/2$, and we have shown that the opening of a gap is associated to a spontaneous dimerization or trimerization depending on the value of $m$ and $N$. We have also investigated the marginal cases where abelian bosonization did not lead to any prediction. In these cases, variational Monte-Carlo predicts that the ground state is critical with exponents consistent with conformal field theory.

I. INTRODUCTION

The SU(N) Heisenberg model with the same irreducible representation (irrep) at each site describes the Mott insulating phases of the Hubbard model for $N$-color fermions in the large $U/t$ limit. As for the SU(2) case, the connection between the Hubbard and Heisenberg models can be made in the large $U/t$ limit using degenerate perturbation theory in $t/U$. The number of fermions per site $m$ for a Mott phase identifies the local totally antisymmetric irreducible representation of the SU(N) Heisenberg model, each site corresponding to a single-column Young tableau with $m$ boxes. The corresponding Hamiltonian can be written:

$$\hat{H} = \sum_{\langle i,j \rangle} \sum_{\alpha\beta} \hat{a}_{i\alpha}^\dagger \hat{a}_{j\beta} \hat{a}_{j\beta}^\dagger \hat{a}_{i\alpha},$$

where $\hat{a}_{i\alpha}$ ($\hat{a}_{i\alpha}^\dagger$) is a fermionic operator that destroys (creates) a particle of color $\alpha$ on site $i$. For a more detailed derivation of this model, see the appendix A.

This model captures the low-energy physics of multi-color ultra-cold atoms in optical lattices, systems for which remarkable progress has been recently achieved on the experimental side. For instance, the SU(N)-symmetry has been observed in ultracold quantum gas of fermionic $^{128}$Yb and $^{87}$Sr. Another example is the realization of one dimensional quantum wires of repulsive fermions with a tunable number of components.

The SU(N) Heisenberg model with the fundamental representation at each site, which corresponds to the Mott phase with one particle per site, has been investigated in considerable detail over the years. In one dimension, there is a Bethe ansatz solution for all values of $N$, and Quantum Monte Carlo simulations free of minus sign problem have given access to the temperature dependence of correlation functions. In two dimensions, a number of simple lattices have been investigated for a few values of $N$ with a combination of semiclassical, variational and numerical approaches, leading to a number of interesting predictions at zero temperature.

In comparison, the case of higher antisymmetric irreps ($m > 1$) has been little investigated. In 2D, there is a mean-field prediction that chiral phases might appear for large $m$ provided $N/m$ is large enough, and some cases of self-conjugate irreps such as the 6-dimensional rep of SU(4) have been investigated with Quantum Monte Carlo simulations. In 1D, apart from a few specific cases, including more general irreps than simply the totally antisymmetric ones, the most general results have been obtained by Affleck quite some time ago. Applying non-abelian bosonization to the weak coupling limit of the SU(N) Hubbard model, he identified two types of operators that could open a gap: Umklapp terms if $N > 2 m$ and $N/m = 2$, and higher-order operators with scaling dimension $\chi = N(m-1)m^{-2}$ allowed by the $Z_{N/m}$ symmetry if $N/m$ is an integer strictly larger than 2. This allowed him to make predictions in four cases: i) $N/m$ is not an integer: the system should be gapless because there is no relevant operator that could open a gap; ii) $N > 2$ and $N/m = 2$: the system should be gapped because Umklapp terms are always relevant; iii) $N/m$ is an integer strictly larger than 2 and $\chi < 2$: the system should be gapped because there is a relevant operator allowed by symmetry. This case is only realized for $N = 6$ and $m = 2$; iv) $N/m$ is an integer strictly larger than 2 and $\chi > 2$: the system should be gapless because there is no relevant operator allowed by symmetry. The only case where the renormalization group argument based on the scaling dimension of the operator does not lead to any prediction is the marginal case $\chi = 2$, which is realized for two pairs of parameters: $(N = 8, m = 2)$ and $(N = 9, m = 3)$. These predictions are summarized in Table 1. Finally, in all gapless cases, the system is expected to be in the SU(N)$_k$ universality class, with algebraic correlations that decay at long distance with a critical exponent $\eta = 2 - 2/N$.

To make progress on the general problem of the SU(N) Heisenberg model with higher antisymmetric irreps, it would be very useful to have flexible yet reliable numerical methods that would allow to test these predictions.
TABLE I. Summary of the predictions of Refs. 38 and 39 for a representative range of SU(N) with m particles per site. Note that models with \( m = k \) and \( m = N - k \) are equivalent up to a constant. Therefore the light gray shaded region can be deduced from the other cases and does not need to be studied.

| \( N/m \) | Gapless | \( \chi > 2 \) | \( \chi = 2 \) | \( \chi < 2 \) | \( N/m = 2 \) |
|---|---|---|---|---|---|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |

The marginal cases are dealt with in the sixth section, while the fifth one deals with the case where there is no Umklapp process but a relevant operator (\( \hat{a}_{i\alpha} \) and \( \hat{a}^\dagger_{i\alpha} \)). When different colors are involved in \( \tilde{T} \), and as long as there is no term mixing different colors, the Hamiltonian can be rewritten as a direct sum: \( \tilde{T} = \bigoplus_{\alpha=1}^{N} \tilde{T}_\alpha \). Then, for each color, there will be one corresponding unitary matrix \( U^\alpha \) that diagonalizes \( \tilde{T}_\alpha \).

So the new fermionic operators are given by:

\[
\hat{c}_{i\alpha} = \sum_{j=1}^{n} U^\alpha_{ij} \hat{a}_{j\alpha}, \quad \hat{c}^\dagger_{i\alpha} = \sum_{j=1}^{n} U^\alpha_{ji} \hat{a}^\dagger_{j\alpha},
\]

and the trial Hamiltonian can be written in a diagonal basis:

\[
\tilde{T} = \bigoplus_{\alpha=1}^{N} \sum_{i=1}^{n} \omega_{i\alpha} \hat{c}^\dagger_{i\alpha} \hat{c}_{i\alpha}
\]

with \( \omega_{i\alpha} < \omega_{i+1\alpha} \).

In the Mott insulating phase, the system possesses \( nm/N \) particles of each color and exactly \( m \) particles per site. By filling the system with the \( nm/N \) lowest energy states of each color, the resulting wave function contains \( nm \) particles:

\[
|\Psi\rangle = \bigotimes_{\alpha=1}^{N} \bigotimes_{i=1}^{n/N} \hat{c}^\dagger_{i\alpha} |0\rangle = \bigotimes_{\alpha=1}^{N} \bigotimes_{i=1}^{n} \sum_{j=1}^{n} U^\alpha_{ji} \hat{a}^\dagger_{j\alpha} |0\rangle.
\]

A Gutzwiller projector \( P^m_G \) is then applied on \( |\Psi\rangle \) to remove all states with a number of particles per site different from \( m \): \( |\Psi_G\rangle = P^m_G |\Psi\rangle \).

Since the Heisenberg model exchanges particles on neighboring sites, the simplest trial Hamiltonian that allows the hopping of particles and its corresponding Gutzwiller projected wave function are:

\[
\tilde{T}^{\text{Fermi}}_\alpha = \sum_{i=1}^{n} \left( \hat{a}_{i\alpha} \hat{a}^\dagger_{i+1\alpha} + h.c. \right) \rightarrow |\Psi_{G}^{\text{Fermi}}\rangle.
\]

In cases where a relevant or Umklapp operator is present, the ground state is expected to be a singlet separated from the first excited state by a gap, and to undergo a symmetry breaking that leads to a unit cell that can accommodate a singlet. In practice, this means unit cells with \( d = N/m \) sites. To test for possible instabilities, we have thus used wave functions that are ground states of Hamiltonians that creates \( d \)-merization:

\[
\tilde{T}^d_\alpha = \sum_{i=1}^{n} \left( t_i \hat{a}_{i\alpha} \hat{a}^\dagger_{i+1\alpha} + h.c. \right)
\]
Assuming that the mirror symmetry is preserved, the wave functions $|\Psi^d_G(\delta)\rangle$ for dimerization ($d = 2$) and trimerization ($d = 3$) have only one allowed free parameter $\delta$, and the hopping amplitudes in a unit cell are given by:

$$
\begin{cases}
  t_i = 1 - \delta & \text{if } i = d \\
  t_i = 1 & \text{otherwise}.
\end{cases}
$$

To test for a possible tetramerization for SU(8) $m = 2$, since the unit cell contains four sites, one additional free parameter is allowed (still assuming that the mirror symmetry is preserved in the ground state). Therefore, we have used the wavefunction $|\Psi^4_G(\delta_1,\delta_2)\rangle$ with hopping amplitudes defined by:

$$
\begin{cases}
  t_i = 1 - \delta_1 & \text{if } i = 2 \\
  t_i = 1 - \delta_2 & \text{if } i = 4 \\
  t_i = 1 & \text{otherwise}.
\end{cases}
$$

This method is always well defined for periodic boundary conditions when $N/m$ is even. But when $N/m$ is odd, the ground state is degenerate for periodic boundary conditions if the translation symmetry is not explicitly broken, and one has to use anti-periodic boundary conditions for $|\Psi^4_{\text{Fermi}}\rangle$, $|\Psi^d_{\text{Fermi}}(0)\rangle$ ($d = 2, 3$) and $|\Psi^4_{\text{Fermi}}(0,0)\rangle$.

The hope is that if $T$ is wisely chosen, then $|\Psi_G\rangle$ captures correctly the physics of the ground state, i.e., with a good variational wave function, $E_G = \langle \Psi_G | H | \Psi_G \rangle \approx E_0$, the exact ground state energy. To check the pertinence of this statement, we have compared the energies and nearest-neighbor correlations with those computed with ED on small systems with open boundary conditions. In the table TAB. II, one can see, for some systems, the comparison between ED and VMC results for the ground state energy. The nearest-neighbor correlations will be compared in the next sections. Considering the excellent agreement between the two methods for the cluster sizes available to ED, there are good reasons to hope that these Gutzwiller projected wave functions can quantitatively describe the properties of the ground state.

| $N$ | $m$ | $n$ | ED | VMC | Error [%] |
|-----|-----|-----|-----|-----|----------|
| 4   | 2   | 16  | -1.6971 | -1.6916 | -0.33 |
| 4   | 2   | 18  | -1.6925 | -1.6866 | -0.35 |
| 6   | 2   | 15  | -2.7351 | -2.7287 | -0.23 |
| 6   | 3   | 12  | -4.0295 | -4.0261 | -0.08 |
| 6   | 3   | 14  | -4.0162 | -4.0123 | -0.10 |
| 8   | 2   | 12  | -3.1609 | -3.1587 | -0.07 |
| 8   | 2   | 16  | -3.1857 | -3.1828 | -0.09 |
| 9   | 3   | 9   | -6.0960 | -6.0810 | -0.25 |
| 9   | 3   | 12  | -6.1162 | -6.0980 | -0.30 |
| 10  | 2   | 15  | -3.3992 | -3.3919 | -0.21 |

TABLE II. Comparison between the ED and VMC energies per site. The incertitudes on the VMC data are smaller than $10^{-4}$. The relative error is always smaller than 0.35%.

B. Exact diagonalizations

On a given cluster, the total Hilbert space grows very fast with $N$, and the standard approach that only takes advantage of the conservation of the color number is limited to very small clusters for large $N$. Quite recently, two of the present authors have developed a simple method to work directly in a given irrep for the SU($N$) Heisenberg model with the fundamental representation at each site, allowing to reach cluster sizes typical of SU(2) for any $N$. This method can be extended to the case of more complicated irreps at each site, in particular totally antisymmetric irreps, and the exact diagonalization results reported in this manuscript have been obtained along these lines.

III. SU($N$) WITH $m = 1$

In this section, we extend the SU(4) results of Wang and Vishwanath to arbitrary $N$ for $m = 1$ (fundamental representation), and we perform a systematic comparison with Bethe ansatz and Quantum Monte-Carlo (QMC) results. Since these systems are known to be gapless, $|\Psi^4_{\text{Fermi}}\rangle$ is the only relevant wave function to study.

![Variational energy per site of SU(N) chains with the fundamental irrep at each site (dots) compared to Bethe ansatz exact results (solid line) and polynomial approximations in 1/N (dashed lines).](image)

FIG. 1. Variational energy per site of SU($N$) chains with the fundamental irrep at each site (dots) compared to Bethe ansatz exact results (solid line) and polynomial approximations in 1/N (dashed lines).

Let us start with the ground state energy. Using Bethe ansatz, Sutherland derived an exact formula for the ground state energy per site $e_0(N)$ that can be written as a series in powers of 1/N:

$$
e_0(N) = -1 + 2 \sum_{k=2}^{\infty} \frac{(-1)^k \zeta(k)}{N^k}
$$

where $\zeta(k) = \sum_{n=1}^{\infty} (1/n^k)$ is Riemann’s zeta function. $e_0(N)$ is depicted in FIG. 1 as a continuous line. The
dashed lines are approximations obtained by truncating the exact solution at order \( N^{-k} \), \( k \geq 2 \). For comparison, the variational energies obtained in the thermodynamic limit after extrapolation from finite size systems are shown as dots in FIG. 1. The agreement with the exact solution is excellent for all values of \( N \), and it improves when \( N \) increases (see table TAB. III). Quite remarkably, the variational estimate is better than the \( N^{-4} \) estimate even for \( SU(3) \).

\[
\begin{array}{|c|c|c|}
\hline
N & BA & VMC \\
\hline
3 & -0.7052 & -0.7007 \\
4 & -0.8251 & -0.8234 \\
5 & -0.8847 & -0.8833 \\
6 & -0.9183 & -0.9173 \\
7 & -0.9391 & -0.9383 \\
8 & -0.9528 & -0.9522 \\
9 & -0.9624 & -0.9620 \\
\hline
\end{array}
\]

TABLE III. Comparison of the variational energies for \( m = 1 \) systems obtained for infinite chains with exact Bethe ansatz. The incertitudes on the VMC data are smaller than \( 10^{-4} \).

We now turn to the diagonal correlations and its associated structure factor defined by (A1) and (A3). At very low temperature, QMC has been used by Frischmuth \emph{et al.} \cite{43} for \( SU(4) \) and by Messio and Mila \cite{44} for various values of \( N \) to compute this structure factor. The QMC data of Messio and Mila and the results obtained with VMC for \( n = 60 \) sites are shown in FIG. 2. Qualitatively, the agreement is perfect: VMC reproduces the singularities typical of algebraically decaying long-range correlations. But even quantitatively the agreement is truly remarkable, and, as for the ground state energy, it improves when \( N \) increases. Clearly, Gutzwiller projected wave functions capture the physics of the \( m = 1 \) case very well.

![FIG. 2. Comparison of the structure factors calculated with VMC (empty squares) and QMC (filled circles) for various SU(N) systems. In the VMC calculations, anti-periodic boundary conditions have been used for SU(3) and SU(5), and periodic ones for SU(4).](image)

IV. \( SU(N) \) WITH \( m = N/2 \)

For these systems, there is a self-conjugate antisymmetric representation of \( SU(N) \) at each site. The ground states of such systems, referred to as extended valence bound solids \cite{45}, are predicted to break the translational symmetry, to be two-fold degenerate and to exhibit dimerization since only two sites are needed to create a singlet, and the spectrum is expected to be gapped.

We have investigated two representative cases, \( (N = 4, m = 2) \) and \( (N = 6, m = 3) \), with ED up to 18 and 14 sites respectively, and the cases \( N = 4 \) to 10 with VMC. The main results are summarized in FIG. 3.

![FIG. 3. ED and VMC results for various SU(N) models with \( m = N/2 \). Upper left panel: size dependence of the energy gap for \( SU(4) \) and \( SU(6) \). Upper right panel: optimal variational parameter \( \delta \) for periodic boundary conditions for \( SU(4) \), \( SU(6) \), \( SU(8) \), and \( SU(10) \). Lower panels: energy per bond for \( SU(4) \) (left) and \( SU(6) \) (right) calculated with ED (circles) and VMC (squares) for open boundary conditions. Note that the optimal variational parameters \( \delta_{\text{opt}} \) are different in the upper right panel and in the lower panels because they correspond to different boundary conditions (periodic and open).](image)
Let us now turn to the the VMC results. Since the relevant instability is a spontaneous dimerization, it is expected that the dimerized $|\Psi_G^{\text{Fermi}}(\delta)|$ wave function allows one to reach lower energy than the $|\Psi_G^{\text{Fermi}}(0)|$ one. This is indeed true for all cases we have investigated (up to $N = 10$ and to $n \gtrsim 100$), and the optimal value of the dimerization parameter $\delta_{\text{opt}} > 0$ is nearly size independent and increases with $N$ (see upper right panel of FIG. 3), in qualitative agreement with the gap increase between SU(4) and SU(6) observed in ED. To further benchmark the Gutzwiller projected wave functions for these cases, we have calculated the bond energy using the optimal value of $\delta$ (open symbols in the lower panel of FIG. 3) for the same clusters as those used for ED with open boundary conditions. The results are in very good quantitative agreement.

With the large sizes accessible with VMC, it is also interesting to calculate the diagonal structure factor. All the structure factors peak at $k = \pi$, but, unlike in the case of the fundamental representation, there is no singularity but a smooth maximum (see FIG. 4). This shows that the antiferromagnetic correlations revealed by the peak at $k = \pi$ are only short range, and that the correlations decay exponentially at long distance, in agreement with the presence of a gap, and with the spontaneous dimerization.

To summarize, ED and VMC results clearly support Affleck’s predictions that the $N/m = 2$ systems are gapped and point to a very strong spontaneous dimerization.

V. SU(6) WITH $m = 2$

This case is a priori more challenging to study because the relevant operator that is generated in the renormalization group theory appears at higher order than the one-loop approximation. Therefore, the gap can be expected to be significantly smaller than in the previous case. This trend is definitely confirmed by ED performed on clusters with up to 15 sites: the gap decreases quite steeply with the system size (see upper left panel of FIG. 5). It scales smoothly however, and a linear extrapolation points to a gap of the order $\Delta E \simeq 0.2$, much smaller than in the SU(6) case with $m = 3$ ($\Delta E \simeq 4$), but finite. On the largest available cluster, the bond energy has a significant dependence on the bond position, with an alternance of two very negative bonds with a less negative one.

These trends are confirmed and amplified by VMC. Indeed, the trimerized wave function $|\Psi_G^{\text{Fermi}}(\delta)|$ leads to a better energy for all sizes, and the optimal value scales very smoothly to a small but finite value $\delta_{\text{opt}} \approx 0.03$. This value is about an order of magnitude smaller than the SU(6) case with $m = 3$, but the fact that it does not change with the size beyond 50 sites is a very strong indication that the system trimerizes (by contrast to the marginal case shown in FIG. 9). The trimerization is confirmed by the lower plots. For $n = 15$, the VMC results are again in nearly perfect agreement with ED, and for $n = 60$, the bond energy shows a very clear trimerization.

To test the nature of the long-range correlations is of course more challenging than in the previous case since a small gap implies a long correlation length. And indeed, on small to intermediate sizes, the structure factor has a sharp peak at $k = 2\pi/3$ very similar to the SU(3), $m = 1$ case (see FIG. 6). However, going to very large system sizes (up to $n = 450$ sites), it is clear that the concavity changes sign upon approaching $k = 2\pi/3$ (see upper right panel of FIG. 6), consistent with a smooth peak,
VI. MARGINAL CASES: SU(8) WITH $m = 2$ AND SU(9) WITH $m = 3$

These two systems are the only ones which possess operators with scaling dimension $\chi = 2$. They are therefore the only cases where it is impossible to predict whether the system is algebraic or gapped on the basis of Affleck’s analysis. As far as numerics is concerned, these cases can again be expected to require large system sizes to conclude.

The ED results are quite similar to the previous case. The scaling of the gap is less conclusive because the last three points build a curve that is still concave and not linear like in the previous case (see the upper right panel of FIG. 7). So one can only conclude that if there is a gap, it is very small, especially for SU(8) with $m = 2$. The bond energies build a pattern which is consistent with a weak tetramerization for SU(8) with $m = 2$, and with a significant trimerization comparable to the SU(6), $m = 2$ case for SU(9) $m = 3$.

The VMC method turns out to give a rather different picture however. For SU(8) with $m = 2$, two variational wave functions ($|\Psi^{\text{Fermi}}_G\rangle$, $|\Psi^1_G(\delta_1, \delta_2)\rangle$) can be tested. Interestingly, for $n = 16$ with open boundary conditions, $|\Psi^\text{Fermi}_G\rangle$ fails to reproduce the bound energies pattern observed with ED but $|\Psi^1_G(0.054, -0.036)\rangle$ is successful (see the upper right panel of FIG. 7). Therefore $|\Psi^\text{Fermi}_G\rangle$ is believed to be the best variational wavefunction. The conclusion is that there is no tetramerization, and that the correlations must be algebraic. This is also supported by the structure factor, which seems to have a singularity at $k = \pi/2$ (see FIG. 8).

Let us now turn to SU(9) with $m = 3$. This system could in principle be trimerized, and therefore $|\Psi^\text{Fermi}_G\rangle$ and $|\Psi^2_G(\delta)\rangle$ have been compared. For small clusters, there is a large optimal value of $\delta$, actually much larger than for SU(6) with $m = 2$, and the bond energies are typical of a strongly trimerized system, in agreement with ED. However, $\delta_{\text{opt}}$ decreases very fast with $n$ until it vanishes for $n \gtrsim 100$ whereas, for SU(6) with $m = 2$, $\delta_{\text{opt}}$ levels off at a finite value beyond $n = 60$ (see FIG. 9). We interpret this behavior as indicating the presence of
a cross-over: on small length scales, the system is effectively trimerized, but this is only a short-range effect, and the system is in fact gapless with, at long-length scale, algebraic correlations.

One can again calculate the structure factor using the best variational wave function (in both cases $|\Psi_G^{\text{Fermi}}\rangle$ for big enough systems) to check if a discontinuity exists. The results displayed in the upper plots of FIG. 8 clearly show a discontinuity at $k = \pi/2$ for the SU(8) and at $k = 2\pi/3$ for SU(9). These discontinuities indicate an algebraic decay of the long-range correlations. The lower plot shows that even if these systems are gapless, there is a maxima of the correlation every $N/m$ sites.

VII. EXAMPLE WITH IRRELEVANT OPERATOR: SU(10) WITH $m = 2$

For completeness, we have also looked at a case where there is an irrelevant operator of scaling dimension larger than 2, namely SU(10) with $m = 2$. As expected, the best variational wave function is $|\Psi_G^{\text{Fermi}}\rangle$ for all sizes, and the structure factor exhibits discontinuities at $k = 2\pi/5$, consistent with a gapless spectrum and algebraic correlations.

VIII. CRITICAL EXPONENTS

Motivated by the remarkably accurate result obtained by Wang and Vishwanath for SU(4) with the fundamental irrep at each site\textsuperscript{14}, we have tried to use the VMC results to determine the critical exponent that controls the decay of the correlation function (A2) at long distance. For periodic boundary conditions, one can use the following fitting function with four free parameters\textsuperscript{7}:

$$c_0(r^{-\nu} + (n-r)^{-\nu}) + c_k \cos(2\pi m/N)(r^{-\eta} + (n-r)^{-\eta})$$

the amplitudes $c_0$ and $c_k$ of the components at $k = 0$ and $k = 2\pi m/N$, and their critical exponents $\nu$ and $\eta$.

The critical exponents $\eta$ are shown in FIG. 10. The theoretical values of the critical exponents $\eta = 2 - 2/N$ are shown as straight lines. In all cases, the extracted exponents agree quite well with the theoretical predictions when $n$ is large enough. In particular, for a given $N$, the exponent $\eta$ does not depend on $m$, as predicted by non-abelian bosonization. The critical exponents $\nu$ has also been extracted but, as already observed\textsuperscript{7}, a precise estimate is difficult to get. Nevertheless, for $N = 3, 4, \nu \in [1.8, 2.25]$ and for $N \geq 5, \nu \in [1.95, 2.05]$ for the largest systems.

FIG. 9. Energy per site as a function of the variational parameter $\delta$ for the SU(6) with $m = 2$ (left) and SU(9) with $m = 3$ (right).

FIG. 10. Critical exponents $\eta$ of the gapless systems as a function of the system size. The squares, circles and triangles correspond respectively to $m = 1, 2,$ and $3$ particles per site. All values given here have been calculated with $|\Psi_G^{\text{Fermi}}\rangle$. 
There is a large degree of freedom in the choice of the fitting range. One could in principle select any arbitrary range of sites \([x_i, x_f]\), \(0 \leq x_i < x_f \leq n - 1\). The problem is that each range will give different critical exponents. In order to obtain some meaningful results the following method has been chosen. Using the periodicity of the systems, only the ranges with \(x_i = a\) and \(x_f = n - a - 1\), \(1 \leq a \leq n/2\) have been considered. For each value of \(a\), the coefficient of determination of the fit has been computed and if its value is higher than 0.999 than the range \([a, n - a - 1]\) is selected to perform the extrapolation of the critical exponents. If the value is too low, the fit is considered to be bad and the range with \(a \leftarrow a + 1\) is tested. If no good range can be found with this criterion, the condition over the coefficient of determination is relaxed to be higher than 0.995 and the first fit with a residual sum of squares divided by \(n\) that is smaller than \(10^{-7}\) is selected.

IX. CONCLUSIONS

Using variational Monte Carlo based on Gutzwiller projected wave functions, we have explored the properties of SU(N) Heisenberg chains with various totally antisymmetric irreps at each site. In the case of the fundamental representation, which is completely understood thanks to Bethe ansatz and to QMC simulations, these wave functions are remarkably accurate both regarding the energy and the long-range correlations. In the case of higher antisymmetric irreps, field theory arguments are in most cases able to predict that the system should be gapless or gapped, allowing for a symmetry breaking term in the tight binding Hamiltonian used to define the unprojected wave function leads to results in perfect agreement with these predictions, and the ground state is found to be spontaneously dimerized or trimerized. Finally, in the two cases where the operator that could open a gap is marginal, SU(8) with \(m = 2\) and SU(9) with \(m = 3\), this variational approach predicts that there is no spontaneous symmetry breaking, and that correlations decay algebraically. These results suggest that the operators are marginally irrelevant in both cases. It would be interesting to test these predictions either analytically by pushing the renormalization group calculations to higher order, or numerically with alternative approaches such as DMRG or QMC.

In any case, these results prove that Gutzwiller projected fermionic wave functions do a remarkably good job at capturing quantum fluctuations in one-dimensional SU(N) Heisenberg models with totally antisymmetric irreps. Considering the encouraging results obtained in 2D for the SU(N) Heisenberg model with the fundamental irrep at each site on several lattices, one can legitimately hope these wave functions to be also good for the SU(N) Heisenberg model with totally antisymmetric irreps at each site in 2D. Work is in progress along these lines.

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Appendix A: SU(N) Heisenberg model

The \(N^2 - 1\) generators of the SU(N) algebra, labelled \(S^\alpha\), can be combined to create new operators, \(\hat{S}_{\alpha\beta}\), satisfying the following commutation relation:

\[
[\hat{S}_{\alpha\beta}, \hat{S}_{\mu\nu}] = \delta_{\mu\beta} \hat{S}_{\alpha\nu} - \delta_{\alpha\nu} \hat{S}_{\mu\beta}
\]

For the totally antisymmetric irreducible representation, they can be expressed with fermionic operators \(\hat{a}_\alpha^\dagger\) and \(\hat{a}_\alpha\):

\[
\hat{S}_{\alpha\beta} = \hat{a}_{\alpha}^\dagger \hat{a}_{\beta} - \frac{m}{N} \delta_{\alpha\beta}
\]

where \(m\) is the number of particles per site. This representation can be labelled by a Young tableau with \(m \leq N\) boxes in one column. For any allowed \(m\), there is a conjugate equivalent representation: a system with \(m = k\) particles per site is equivalent to a system with \(m = N - k\) particles per site.

With this formulation, the SU(N) Heisenberg Hamiltonian that acts on neighbouring sites \(i\) and \(j\) is given by:

\[
\hat{H} = \sum_{<i,j>} \sum_{\alpha \beta} \hat{S}_{\alpha\beta}^i \hat{S}_{\beta\alpha}^j - \sum_{<i,j>} \sum_{\alpha \beta} \hat{a}_{i\alpha}^\dagger \hat{a}_{j\beta} \hat{a}_{j\alpha}^\dagger \hat{a}_{i\alpha} - \frac{m z}{2 N}
\]

where \(n\) is the total number of particles and \(z\) is the coordination number. For one particle per site, this Hamiltonian corresponds, up to a constant term, to a permutation Hamiltonian.

The long-range diagonal correlation is defined by:

\[
C(r) = \sum_{\alpha} \langle \hat{S}_{\alpha\alpha}^i \hat{S}_{\alpha\alpha}^r \rangle = \sum_{\alpha} \langle \hat{a}_{\alpha\alpha}^\dagger \hat{a}_{\alpha\alpha} \rangle \frac{m^2}{N} - \frac{m z}{2 N}
\]

For the particular case of gapless systems, conformal field theory predicts an algebraic decay of the long-range correlations function according to:

\[
C(r) = \frac{c_\eta}{r^2} + \frac{c_k \cos (2\pi r m / N)}{r^\eta}
\]

where \(\eta = 2 - 2/\nu\) is the critical exponent. The structure factor is the Fourier transform of the long-range correlations:

\[
\tilde{C}(k) = \frac{1}{2\pi \eta m (N - m)} \sum_r C(r) e^{ikr}
\]

where the prefactor has been chosen such that:

\[
\sum_k \tilde{C}(k) = \frac{n}{2\pi}
\]
