Stabilization of the chiral phase of the SU(6m) Heisenberg model on the honeycomb lattice with m particles per site for m larger than 1

Jérôme Dufour and Frédéric Mila
Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland
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We show that, when N is a multiple of 6 (N = 6m, m integer), the SU(N) Heisenberg model on the honeycomb lattice with m particles per site has a clear tendency toward chiral order as soon as m ≥ 2. This conclusion has been reached by a systematic variational Monte Carlo investigation of Gutzwiller projected wave-functions as a function of m between the case of one particle per site (m = 1), for which the ground state has recently been shown to be in a plaquette singlet state, and the m → ∞ limit, where a mean-field approach has established that the ground state has chiral order. This demonstrates that the chiral phase can indeed be stabilized for not too large values of m, opening the way to its experimental realisations in other lattices.

I. INTRODUCTION

Progress in cold atoms experiments has opened the door to new and exciting physics1–7. When fermionic ultracold alkaline-earth atoms with nuclear spin I are trapped in optical lattices, the physics is governed by a generalized Hubbard model with N = 2I + 1 colors (or flavors) of fermionic particles8–11. In the limit of strong on-site repulsion, when the optical wells are deep, and if the number of atoms per site is an integer, this system is in a Mott insulating phase and the low energy physics is effectively described by the SU(N) Heisenberg model:

\[ \hat{H} = \sum_{<i,j>} \sum_{\alpha\beta} S^\alpha_i \delta^\beta_j. \] (1)

This Hamiltonian is known to exhibit various ground states depending not only on the lattice but also on the number of colors N and on the on-site SU(N) symmetry of the wave function, i.e. the irreducible representation (irrep) labelled by a Young tableau with m boxes. For ultra-cold fermions, the case of m atoms per well corresponds to the fully antisymmetric irrep with a Young table of one column with m boxes: a non-exhaustive list of exotic ground states contains tableau consisting of a single column with m boxes representing the fully antisymmetric irrep with a Young tableau with m boxes in one column:

\[ \text{SU}(6) \quad \text{SU}(12) \quad \text{SU}(18) \ldots \]

For this family of irreps, the fermionic operators \( \hat{c}^\dagger, \hat{c} \) together with the identity:

\[ \hat{S}^\alpha = \hat{c}^\dagger_\alpha \hat{c}_\beta - \frac{m}{N} \delta_{\alpha\beta} \] (2)

allow the rewriting of Eq.1 as:

\[ \hat{H} = \sum_{<i,j>} \sum_{\alpha\beta} \hat{c}^\dagger_{i\alpha} \hat{c}_{j\beta} - \frac{m}{N} \delta_{\alpha\beta} \hat{c}_{i\alpha} \hat{c}_{j\beta} \hat{c}^\dagger_{i\alpha} \hat{c}_{j\beta} \] (3)
where the constant $-zm^2/2N$ has been dropped. In
the following, our goal is to investigate how the system
evolves between the chiral ground state of Ref.[29] for
$m = \infty$ and the $0\pi\pi$ plaquette ground state of Ref.[32]
obtained for $m = 1$. We will present numerical results
that give strong indication that the chiral phase is stabi-
lized for $m > 1$.

II. VMC RESULTS

A. Method

Since our aim is to systematically study the fully anti-
symmetric irreps of the SU(6m) Heisenberg model on
the honeycomb lattice, we need a numerical method
that works for any $m$. Quantum Monte Carlo suffers
from the sign problem, ED does not give access to large
enough clusters when $m > 1$, and iPEPS has so far only
given results for $m = 1$. The variational Monte Carlo
(VMC) method is therefore the only reliable numerical
method that was proven to be efficient to study
more complicated representations like the fully anti-
symmetric irreps. It is not limited by the system size
and recovers the mean-field results when $N$ and $m$ are
large.

To have meaningful results we need to define a rep-
resentative set of variational wave functions. Following
other papers and inspired by the mean-field results[29],
we have tested five different variational wave functions
represented in FIG. 1, one chiral and four plaquette
states. The chiral wave function is the only one having
no variational parameter. It has uniform hopping ampli-
ditudes but non-uniform phase factors that creates a homo-
genous flux of $2\pi/3$ per hexagonal plaquette. This wave
function does not break the lattice symmetry but breaks
the time reversal one. We want the other wave functions
to preserve the time reversal symmetry, therefore the only
allowed fluxes are 0 and $\pi$. To preserve the rotation sym-
mmetry, and since we chose unit cells containing at most
12 sites, there are only 4 non-equivalent flux configura-
tions. Two of them have already been introduced, 000
and 000, while the other two are: $\pi00$ consisting of a cen-
tral hexagon with $\pi$ flux surrounded by 0 fluxes and $\pi\pi\pi$
having a homogeneous $\pi$ flux in each hexagon. Due to
the simplicity of the chosen flux configurations, there are
only two meaningful variational parameters, $t_h$ and $t_d$:
the hopping terms around the central hexagons $t_h$, and
the hopping terms linking these hexagons $t_d$. Using addi-
tional hopping terms would break other symmetries, for
instance having different hopping terms around the cen-
tral hexagon would break the rotational symmetry. Since
the honeycomb lattice is bipartite, only the relative sign
of $t_d$ and $t_h$ matters, therefore, for the plaquette wave
functions, we have a single variational free parameter,
the ratio $t_d/t_h$ with fixed $t_h = -1$.

FIG. 1. Representation of the five wave functions with their
unit cell on a 24-site cluster with periodic boundary condi-
tions. (a)-(b) Plaquette wave functions, where solid blue and
dashed green bonds stand for $t_h$ and $-t_h$ respectively, while
the thin yellow ones stand for $t_d$. By changing the sign of the
ratio $t_d/t_h$ from negative to positive, the flux configuration
of the wave function will change from $\pi00$ to $\pi\pi\pi$ in (a)
and from $0\pi\pi$ to 000 in (b). (c) Chiral wave function for which the
hopping terms are given by $t_{ij} = t_h e^{i2\pi/3} = t_{ij}^*$ between
the sites $i$ and $j$ connected by a red arrow and by $t_h$ otherwise.
The flux per plaquette is defined mod $2\pi$.

B. Results

In this section, results on a 72-site cluster with anti-
periodic boundary conditions will first be presented.
Then a finite size analysis on a representative example,
$m = 3$, will show how accurately the thermodynamic
energies can be extracted. This accuracy allows us to
draw conclusions on how the VMC recovers the mean-
field limit and gives new indications of a chiral phase for
$m > 1$.

FIG. 2 shows the variational energies as a function of
$m$ for different values of the ratio $t_d/t_h$ for all differ-
et wave functions on a 72-site cluster with anti-periodic
boundary condition. This particular choice of boundary
conditions allows us to measure the energy for $t_d/t_h = -1$
because it lifts the well-known degeneracy at the Fermi
level, an important requirement to construct Gutzwiller
projected wave functions. However, it does not lift the
degeneracy for the value $t_d/t_h = 1$. The other missing
energy is for $t_d/t_h = 0$ because the VMC fails to find a
well defined starting configuration, since all hexagons are
disconnected. On the lowest plot, the chiral energies are
also shown as straight lines.

We can see that each plaquette wave function has at
least one local minimum. While the exact position of the
minima does not really matter, it is interesting to note
that for all wave functions but the 000 one, the minima
stay roughly stable. Indeed, we know that the 000 mean-
field solution consists of disconnected hexagons with 0
flux. This solution is expected to be captured by the 000
variational wave function, when $m$ is going to infinity
for a small value of $t_d/t_h$. This is indeed what can be
observed in the lower plot of FIG. 2: the position of the
000 minimum moves to the left when $m$ increases but
the value of its energy remains higher than the energy of
both the $0\pi\pi$ and the chiral wave function. By looking
more carefully at the energies of the chiral and $0\pi\pi$ wave

\begin{align*}
\text{energy} &= -z(m^2/2N) + z \sum_{ij} t_{ij} \epsilon_i - \frac{1}{2} \sum_{ij} t_{ij} \epsilon_i \epsilon_j,
\end{align*}

where $z$ is the number of sites in the unit cell, and $\epsilon_i$ is
the energy at site $i$. This equation is the Hamiltonian of
the system in the mean-field approximation. The variational
wave functions are represented by wave functions of the
form

\begin{align*}
\psi(t_h, t_d) &= \prod_{i,j} \left( 1 + B(t_h, t_d) \phi_{ij} \right),
\end{align*}

where $B(t_h, t_d)$ is a matrix element that depends on
the hopping parameters $t_h$ and $t_d$. The variational
wave functions are then used to calculate the variational
energy

\begin{align*}
\mathcal{E}(t_h, t_d) &= -z(m^2/2N) + z \sum_{ij} t_{ij} \epsilon_i - \frac{1}{2} \sum_{ij} t_{ij} \epsilon_i \epsilon_j.
\end{align*}

The variational energy is then minimized with respect to
the two hopping parameters $t_h$ and $t_d$. This results in
the following equations

\begin{align*}
\frac{\partial \mathcal{E}}{\partial t_h} &= 0, \\
\frac{\partial \mathcal{E}}{\partial t_d} &= 0.
\end{align*}

Solving these equations yields the optimal values of $t_h$ and
$t_d$. The variational energy is then compared to the exac
energy to determine how well the variational wave func-
tions describe the ground state of the system.

In FIG. 2, we can see that the variational energy decreases
as $m$ increases. This indicates that the variational wave
functions are getting closer to the true ground state of
the system. The value of $t_d/t_h$ that minimizes the vari-
ational energy is shown as a function of $m$ in the figure.

We can see that the value of $t_d/t_h$ that minimizes the
variational energy decreases as $m$ increases. This indi-
cates that the chiral wave function becomes more impor-
tant as $m$ increases. The value of $t_d/t_h$ that minimizes
the variational energy is shown as a function of $m$ in the
figure.

In summary, we have studied the variational Monte Carlo
method for the SU(6m) Heisenberg model on the honey-
comb lattice. We have found that the chiral wave function
becomes more important as $m$ increases, and that the vari-
ational energy decreases as $m$ increases. These results
provide new indications of a chiral phase for $m > 1$.
functions, it seems that the former becomes lower when $m$ increases and the latter remains stable. This behavior is the most interesting feature of this analysis on a 72-site cluster. Indeed, there is a strong competition between the chiral and $0\pi\pi$ wave functions when $m = 1$ and for $m > 1$ the energy of the chiral wave function becomes clearly lower.

The same study has been done for larger clusters (up to 288 sites) and the energies in the thermodynamic limit have been extrapolated. As an example, FIG. 3 shows the variational energies as a function of the system size for $m = 3$. It is clear that the chiral wave function gives lower energies than any of the plaquette ones no matter what the size of the system is.

The results shown in FIG. 4 are the energies extrapolated in the thermodynamic limit. Let us first focus on already published results for the case with $m = 1$. The chiral and $0\pi\pi$ wave function are in strong competition as already visible in FIG. 2. It was numerically concluded on the basis of extensive ED, VMC and iPEPS calculations\cite{32} that the ground state is the $0\pi\pi$ plaquette state. In the context of our calculation, where we only calculate the energy of a single wave function, the chiral state turns out to have a slightly lower energy, but as shown in Ref.\cite{32}, if several variational wave-functions with differ-
ent boundary conditions are coupled, this small energy difference is reverted in favour of the plaquette phase.

As soon as $m = 2$, the energy of the chiral wave function becomes much lower than the energy of any plaquette wave function, with an energy difference of the same order of magnitude than that of the $m \to \infty$ case. Moreover, this difference increases for larger values of $m$. The results for $m > 1$ can be fitted linearly in $1/m$, and the slope of the fit of the chiral wave function energy is bigger than that of the plaquette wave function. Let us note that the extrapolations of the fits to the limit $m = \infty$ of the three lowest states (chiral, $0 \pi$ and 000 plaquettes) agree with the mean-field energies, a good test of the validity of our VMC simulations.

III. CONCLUSION

We have shown in the context of the SU($N$) model on the honeycomb lattice with $N = 6m$, where $m$ is the number of particles per site, that the presence of chiral order in the mean-field limit ($m \to \infty$) is representative of finite values of $m$ down to $m = 2$. From that point of view, the case $m = 1$ with its plaquette ground state appears as an exception. This is an interesting step forward towards the stabilisation of chiral order in a simple Heisenberg model with only nearest neighbour permutation and no ring-exchange term. The first candidate in order of increasing $N$ is SU(12) $m = 2$. It is still too large to be realized with alkaline rare earths, which are limited to $N \leq 10$, but very close. This result suggests that a systematic investigation of SU($N$) models with $N \leq 10$ for all compatible values of $m$ (i.e. values of $m$ that divide $N$) and different lattice geometries might indeed reveal a case of chiral order that could be stabilized with alkaline rare earths and only nearest-neighbor permutations. Work is in progress along these lines.

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