The mass gap of the 2D O(3) Heisenberg model at $\theta=\pi$ from simulations at imaginary $\theta$

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Haldane, Affleck and others, showed that antiferromagnetic 1D chains of quantum spins present two kinds of large distance correlations: exponentially falling if the spin $\sigma$ is integer and power-law if $\sigma$ is half-integer.

It was also shown that the 1D chain of quantum spins $\sigma$ shares the same large distance physics than the 2D non-linear O(3) sigma model with a theta term $\theta=2\pi\sigma$.

In particular, and due to the periodicity of the topological $\theta$ term, this equivalence should imply that the 2D O(3) non-linear sigma model with a $\theta=\pi$ term must be massless.

Two recent numerical simulations (Bietenholz et al., Azcoiti et al.) suggest that the model undergoes a second order phase transition at $\theta=\pi$.

We have directly calculated the mass gap by numerical simulation.
A direct simulation of the 2D O(3) nonlinear sigma model at $\theta=\pi$ runs with two tough problems:

- if indeed the model is critical then a direct Monte Carlo simulation becomes unfeasible since exponentially large lattice sizes are needed and
- at real $\theta$ the Boltzmann weight is complex and loses its probability meaning.

Then we have simulated the model at imaginary $\theta, \theta = i\vartheta, \vartheta \in \mathbb{R}$, and analytically continued the results to the real $\theta$ axis. The continuation was performed through a numerical extrapolation.

In the simulations we used the standard action,

$$S = A - i\theta L Q, \quad A \equiv -\beta \sum_{x, \mu} \bar{\phi}(x) \cdot \bar{\phi}(x + \mu).$$
As for the topological charge $Q$ we made use of two different definitions on the lattice. We called them $Q^{(1)}$ and $Q^{(2)}$. The first one is the usual naive (also called field-theoretical), the corresponding density of charge being

$$Q^{(1)}(x) = \frac{1}{32\pi} \epsilon^{\mu\nu} \epsilon_{dbc} \phi^d(x) \left( \phi^b(x + \hat{\mu}) - \phi^b(x - \hat{\mu}) \right) \left( \phi^c(x + \hat{\nu}) - \phi^c(x - \hat{\nu}) \right)$$

where $d,b,c$ are O(3) group indices and $\mu,\nu$ are space indices. $Q^{(1)}(x)$ satisfies the continuum limit

$$Q^{(1)}(x) \xrightarrow{a \to 0} a^2 Q(x)$$

$Q(x)$ being the density of topological charge in the continuum.
It is well-known that in general the lattice topological charge must be renormalized, \( Q^{(1,2)} = Z_Q^{(1,2)} Q \), where \( Q \) is the integer-valued continuum charge.

The renormalization constant of the geometrical charge is \( Z_Q^{(2)} = 1 \) (Lüscher). On the other hand \( Z_Q^{(1)} \) depends on \( \beta \) (not on \( \theta \)) and in general is different from 1.

\( Z_Q^{(1)} \) was originally computed in perturbation theory (Campos-trini et al.). We have chosen instead a non-perturbative method to evaluate this constant (Di Giacomo-Vicari).

A configuration with total topological charge \( Q = 1 \) is heated at a temperature \( \beta \) (100 Heat-Bath steps) without changing the topological sector (cooling checks are periodically done). The value of \( Q^{(1)} \) at equilibrium must be \( Z_Q^{(1)} Q = Z_Q^{(1)} \).
\[ Z_Q^{(1)} (\beta = 1.5) = 0.285(9) \]
The relevant consequence of the above considerations for our work is that the $\theta_L$ parameter that appears in the expression of the Hamiltonian used in our computer program in general is not equal to the true physical $\theta$ parameter. They are related by $\theta=\theta_L Z_{Q^{(1,2)}}$. Clearly this distinction only applies to the naive charge $Q^{(1)}$ since $Z_{Q^{(2)}}=1$ for all $\beta$.

Using the lattice topological charge $Q^{(1)}$ (that requires the extra calculation of a renormalization constant) has its advantage…

… $Q^{(1)}$ can be simulated by using a fast cluster algorithm that has been expressly introduced in the present investigation. Thanks to this updating algorithm, the simulation of a single value of $\beta$ with $Q^{(1)}$ is, including the computation of $Z_{Q^{(1)}}$, much faster than the analogous simulation with $Q^{(2)}$. 
Every updating of a cluster algorithm starts by introducing a random unit vector and separating the components parallel and perpendicular to it for all spins (Swendsen-Wang, Wolff),

\[ \tilde{\phi}(x) = \left( \vec{r} \cdot \tilde{\phi}(x) \right) \vec{r} + \tilde{\phi}_\perp(x), \]

where the scalar product is called “equivalent Ising spin”.

Introducing this splitting into the definition of \( Q^{(1)} \), we obtain an expression that is linear in the equivalent Ising spin (because \( Q^{(1)} \) is written in terms of a determinant of three spin vectors).

Therefore the problem turns into an Ising model with site-dependent couplings and within a local magnetic field \( h(x) \),

\[ h(x) \propto \delta_L \left| \vec{r} \cdot \tilde{\phi}(x) \right| \]
There are several algorithms adapted to simulate Ising models in a local magnetic field (Wang, Lauwers-Rittenberg). After testing their performances, we chose the Wang method.

- Our algorithm satisfies the detailed balance property.
- The Fortuin-Kasteleyn clusters were created by using the Hoshen-Kopelman procedure.
- The initial random vector was generated by the Niedermayer method in order to bolster ergodicity.

We extracted the correlation length $\xi$ from the exponential decay of the largest eigenvalue in the matrix of correlation functions among the two operators

\[ O_1 \equiv \vec{\phi}(x) \quad O_2 \equiv \vec{\phi}(x) \times \vec{\phi}(x + \hat{1}) \]
Analytical continuation was performed by a numerical extrapolation.

Polynomials in $\theta_L^2$ and their ratios were used as trial functions.

The Renormalization Group prediction was avoided as a trial function since it assumes the vanishing of $1/\xi$ and we preferred to leave room for any behaviour.
$\beta = 1.5, \, Q^{(1)}$
\[ \frac{c_1 + c_2 \theta_L^2}{1 + c_3 \theta_L^2} \]

<table>
<thead>
<tr>
<th>$\beta$</th>
<th>$L$</th>
<th>$(\theta_{L, \text{zero}})^2$</th>
<th>$Z_{Q}^{(1)}$</th>
<th>$\chi^2$/d.o.f.</th>
<th>$\theta_{\text{zero}}$</th>
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<td>1.75</td>
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<td>56(3)</td>
<td>0.412(5)</td>
<td>0.68</td>
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</table>
\[
\frac{c_1 + c_2 \theta^2}{1 + c_3 \theta^2}
\]

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<tr>
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<th>$L$</th>
<th>$(\theta_{\text{zero}})^2$</th>
<th>$Z_Q^{(2)}$</th>
<th>$\chi^2$/d.o.f.</th>
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<td>9.7(1.0)</td>
<td>1.0</td>
<td>0.73</td>
<td>3.11(16)</td>
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Conclusions

1. We have simulated the O(3) nonlinear sigma model with an imaginary \( \theta \) term, measured the mass gap and extrapolated the results to real \( \theta \) in order to give evidence for the theoretically expected criticality at \( \theta=\pi \).

2. Our results are in excellent agreement with expectations: assuming gaussian errors, our world average for the value of \( \theta \) where the mass gap closes is \( \theta=3.10(5) \).

3. The above number seems very robust since compatible results were obtained by using two different topological charge operators.

4. A fast cluster algorithm was purposely introduced for simulations at imaginary \( \theta \) for one of the two topological charges. The other topological charge operator was simulated by the usual (rather slow) Metropolis updating.