Monte Carlo Evidence of the Haldane Conjecture

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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 σ is integer and power-law if σ is half-integer.
- It was also shown that the 1D chain of quantum spins σ 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 θ 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 $\theta=\pi$, although the two papers disagree in assigning the universality class.
- 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 θ the Boltzmann weight is complex and loses its probability meaning.
- Then we have simulated the model at imaginary θ, $\theta= i\vartheta$, $\vartheta \in \mathbb{R}$, and analytically continued the results to the real θ axis. The continuation was performed by use of a numerical extrapolation.
- In the simulations we used the standard action,

$$S = A - i\theta_L Q, \qquad A \equiv -\beta \sum_{x,\mu} \vec{\phi}(x) \cdot \vec{\phi}(x+\hat{\mu}).$$

- We did not use actions (expansion parameters) with better scaling (asymptotic scaling) since we were interested only in the vanishing of $1/\xi$.

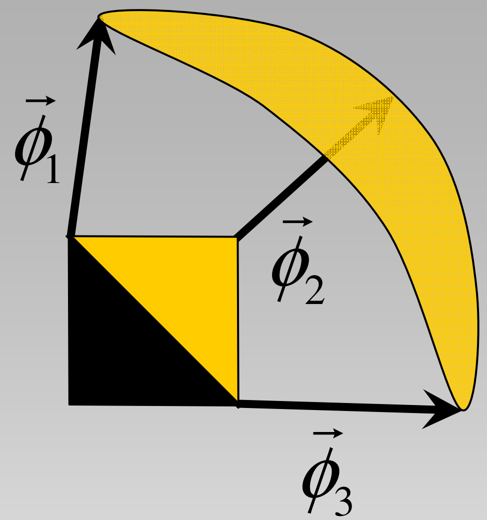
- As for the topological charge Q we made use of two different definitions on the lattice. We called them $Q^{(1)}$ and $Q^{(2)}$. The first one is the usual naive (also called field-theoretical), the corresponding density of charge being

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

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

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

$Q(x)$ being the density of topological charge in the continuum.

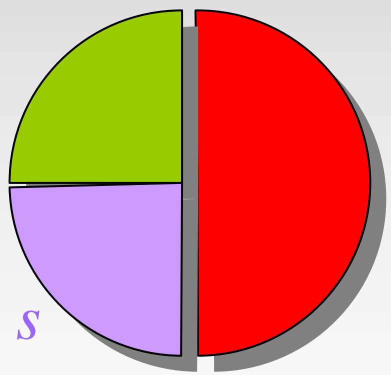


$$c \equiv \cos\frac{Area}{2} = \frac{1}{\rho}\left(1+\vec{\phi}_1\cdot\vec{\phi}_2+\vec{\phi}_2\cdot\vec{\phi}_3+\vec{\phi}_3\cdot\vec{\phi}_1\right)$$

$$s \equiv \sin\frac{Area}{2} = \frac{1}{\rho}\vec{\phi}_1\cdot\left(\vec{\phi}_2\times\vec{\phi}_3\right)$$

$$\rho^2 \equiv 2\left(1+\vec{\phi}_1\cdot\vec{\phi}_2\right)\left(1+\vec{\phi}_2\cdot\vec{\phi}_3\right)\left(1+\vec{\phi}_3\cdot\vec{\phi}_1\right)$$

Area/2=π−arc sin *s*

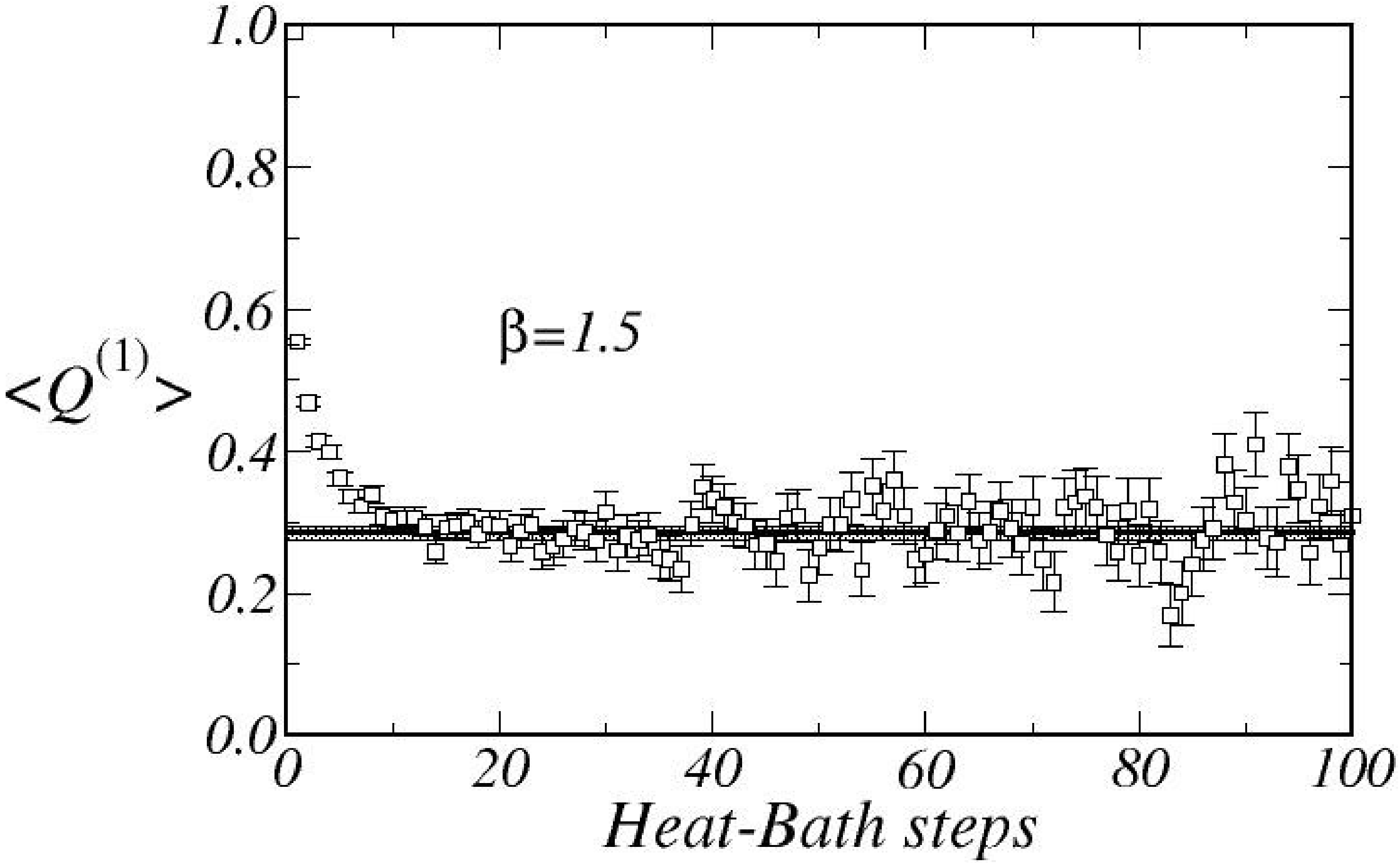


Area/2=arc sin *s*

Area/2=−π−arc sin *s*

$Q^{(2)} = 1/4\pi\, \Sigma\, Area$

- It is well-known that in general the lattice topological charge must be renormalized (Pisa group), $Q^{(1,2)}=Z_Q^{(1,2)}\,Q$, 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 β (not on θ) and in general is different from 1.
- $Z_Q^{(1)}$ was originally computed in perturbation theory (Campostrini 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 β (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 θ_L parameter that appears in the expression of the Hamiltonian used in our computer program in general is not equal to the true physical θ 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 β.

- 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 $Q^{(1)}$ is, even including the computation of $Z_Q^{(1)}$, much faster than the simulation of $Q^{(2)}$.

- 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),

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

where the scalar product is called "equivalent Ising spin".

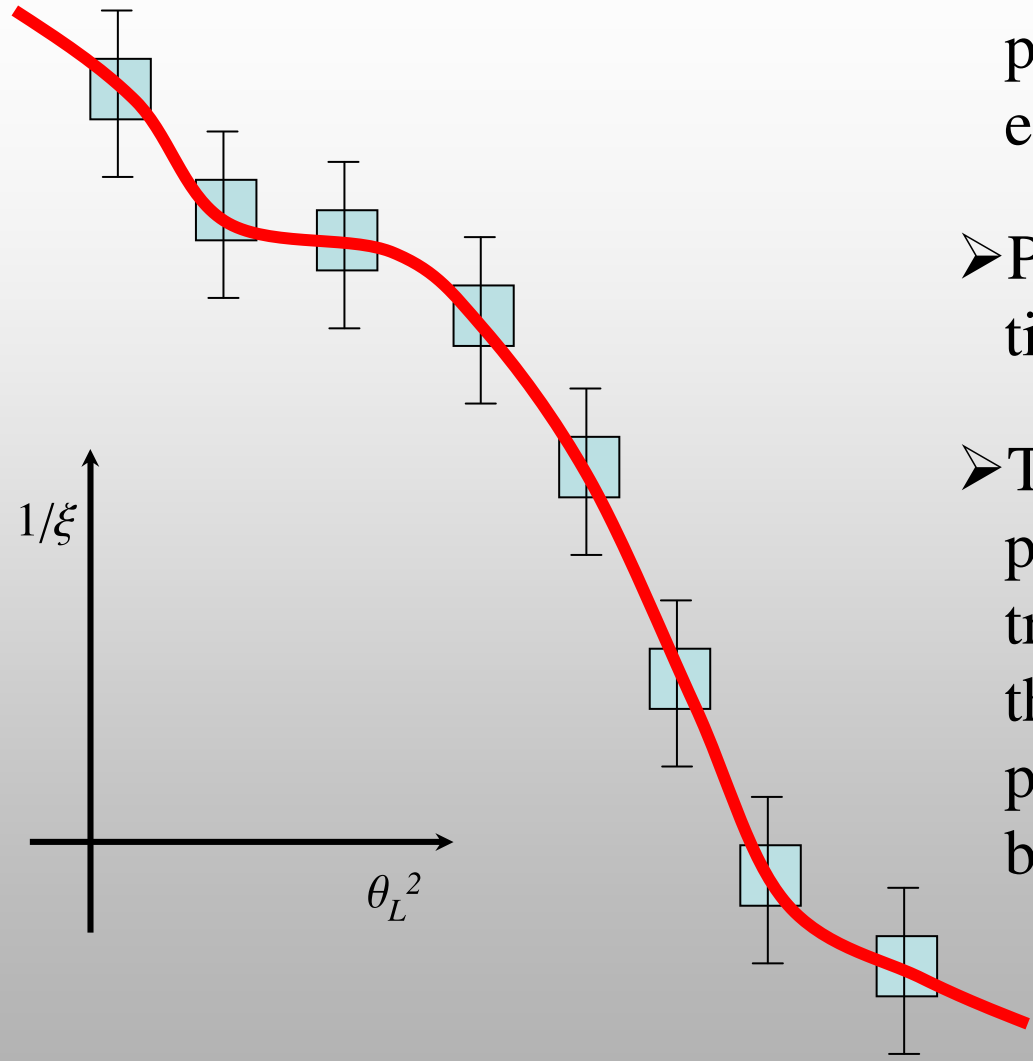
- Introducing this splitting into the definition of $Q^{(1)}$, we obtain an expression that is linear in the equivalent Ising spin (because $Q^{(1)}$ is written in terms of a determinant of three spin vectors).
- Therefore the problem turns into an Ising model with site-dependent couplings and within a local magnetic field *h(x)*,

$$h(x) \propto \vartheta_L \left| \vec{r} \cdot \vec{\phi}(x) \right|$$

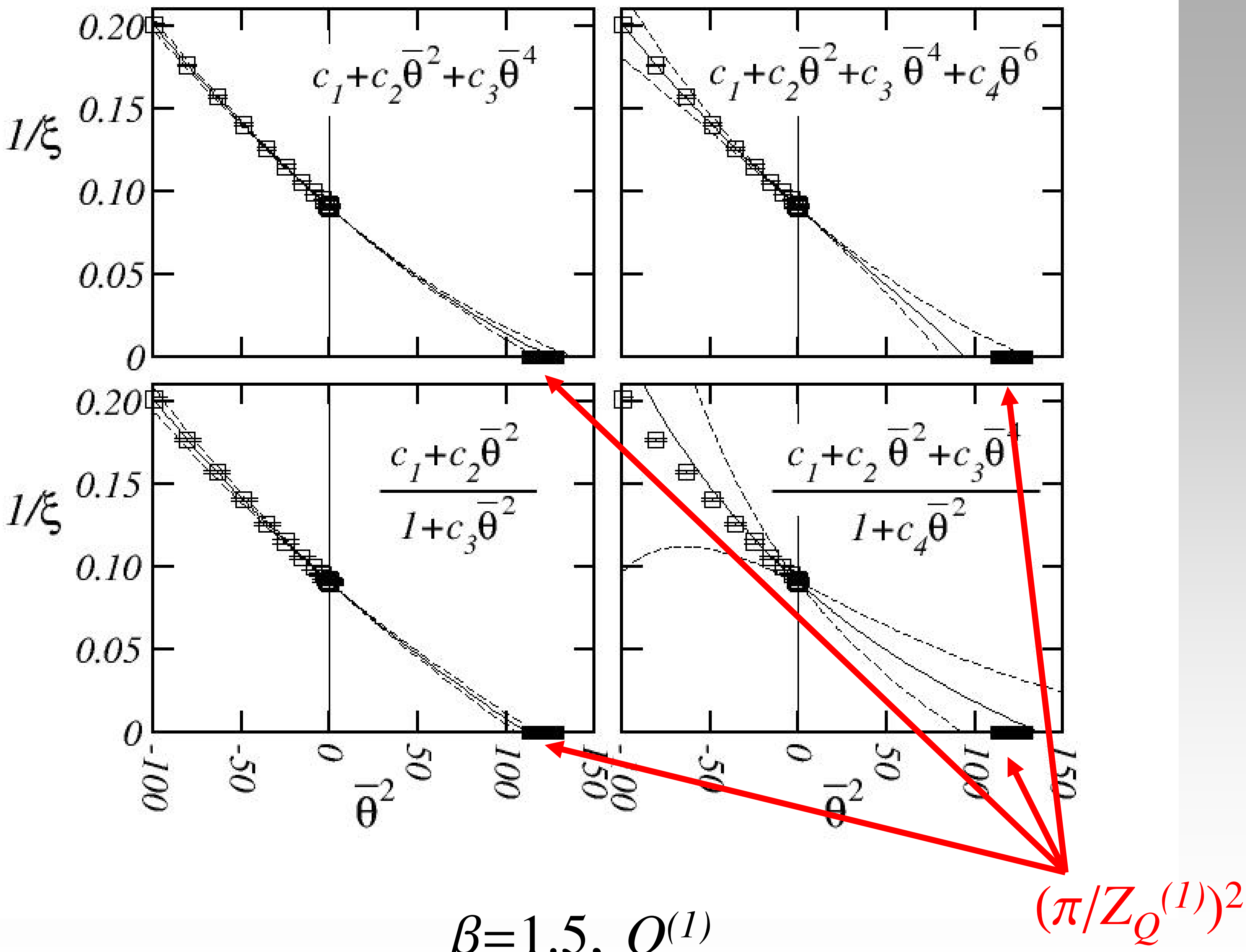
- There are several algorithms adapted to simulate Ising models in a local magnetic field (Wang, Lauwers-Rittenberg). After testing their performances, we chose the Wang method.
  - Our algorithm satisfies the detailed balance property.
  - The Fortuin-Kasteleyn clusters were created by using the Hoshen-Kopelman procedure.
  - The initial random vector was generated by the Niedermayer method in order to bolster ergodicity.

- We extracted the correlation length ξ from the exponential decay of the largest eigenvalue in the matrix of correlation functions among the two operators

$$O_1 \equiv \vec{\phi}(x) \qquad O_2 \equiv \vec{\phi}(x) \times \vec{\phi}(x+\hat{1})$$

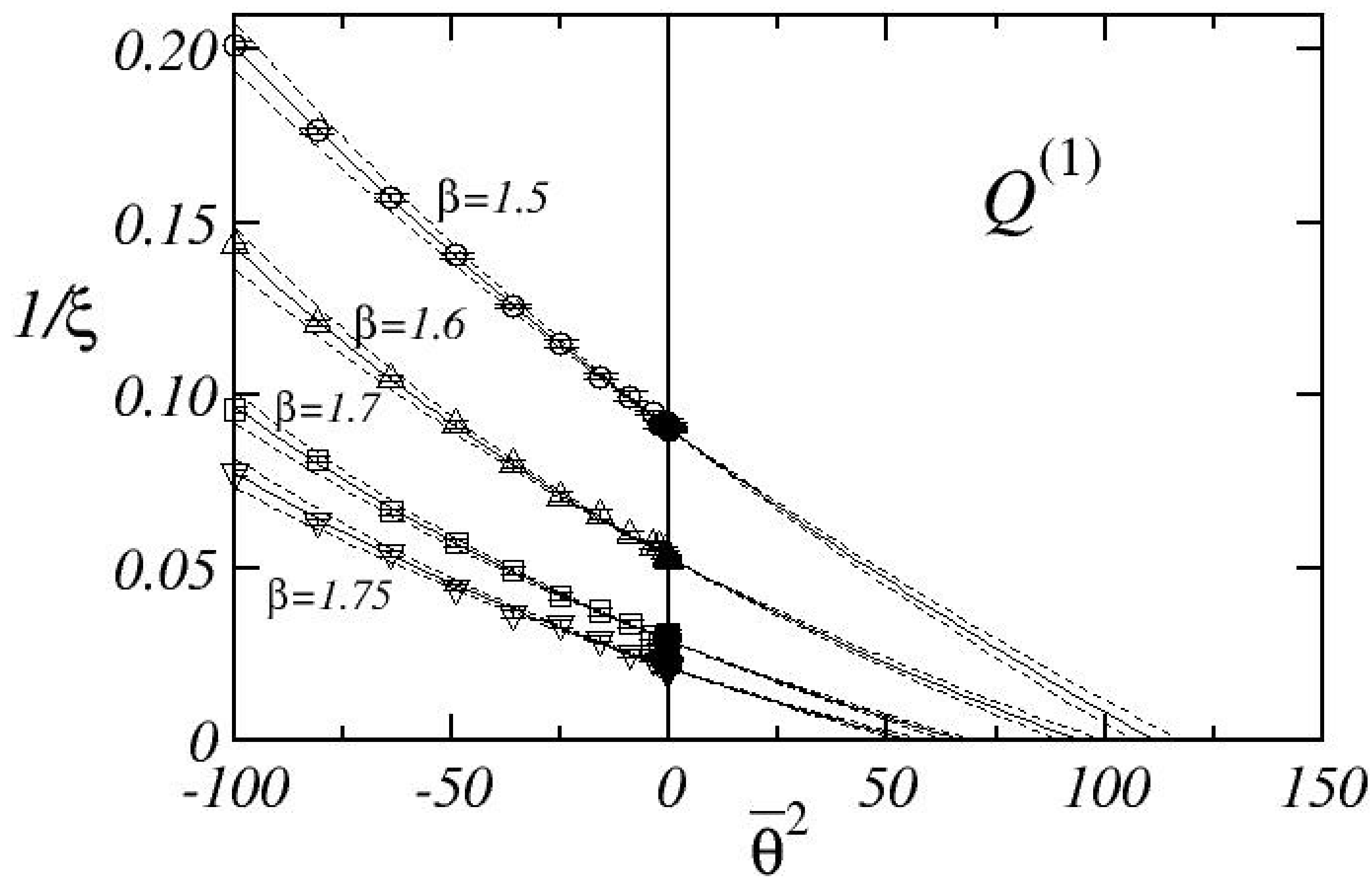


- Analytical continuation was performed by a numerical extrapolation.
- Polynomials in $\theta_L{}^2$ and their ratios were used as trial functions.
- The Renormalization Group prediction was avoided as a trial function since it assumes the vanishing of $1/\xi$ and we preferred to leave room for any behaviour.



$c_1+c_2\bar{\theta}^2+c_3\bar{\theta}^4$
$c_1+c_2\bar{\theta}^2+c_3\bar{\theta}^4+c_4\bar{\theta}^6$
$\frac{c_1+c_2\bar{\theta}^2}{1+c_3\bar{\theta}^2}$
$\frac{c_1+c_2\bar{\theta}^2+c_3\bar{\theta}^4}{1+c_4\bar{\theta}^2}$
$1/\xi$
0.20
0.15
0.10
0.05
0
-100
-50
0
50
100
150
$\bar{\theta}^2$
$(\pi/Z_Q^{(1)})^2$

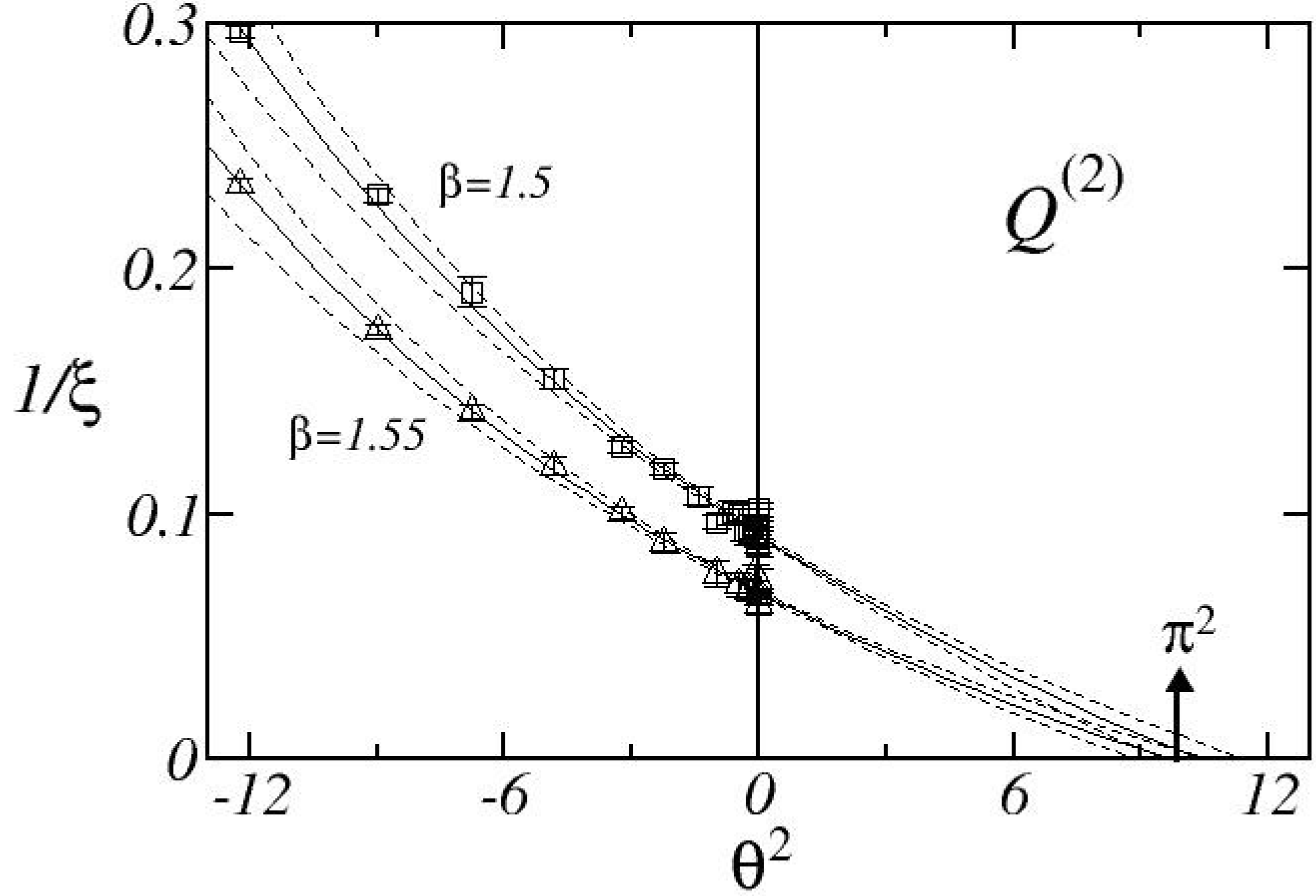
β=1.5, $Q^{(1)}$



0.20
0.15
0.10
0.05
0
1/ξ
β=1.5
β=1.6
β=1.7
β=1.75
Q(1)
-100
-50
0
50
100
150
θ̄²

$$\frac{c_1 + c_2\theta_L^2}{1 + c_3\theta_L^2}$$

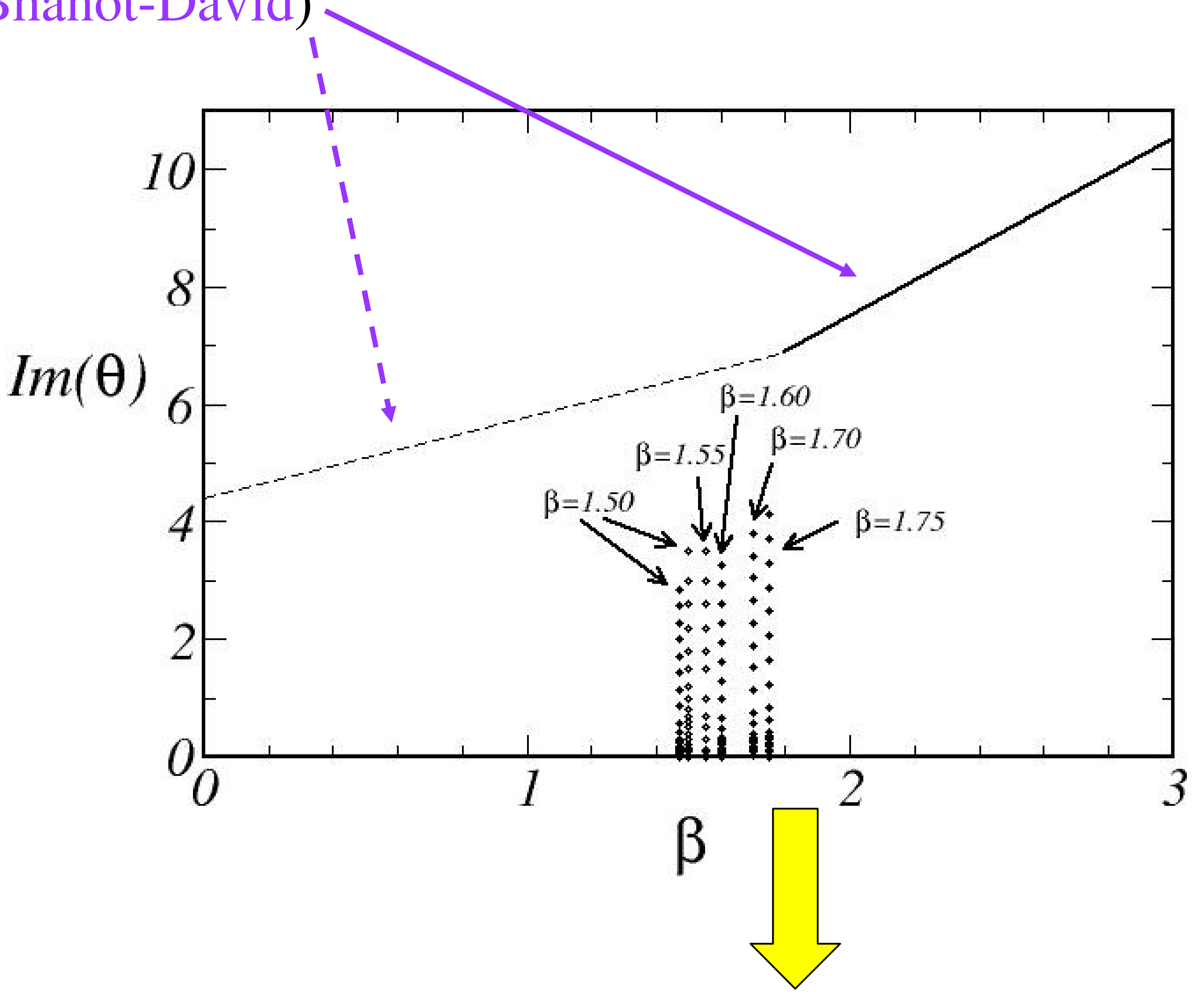
β	$\boldsymbol{L}$	$(\theta_{\mathrm{L,zero}})^2$	$\boldsymbol{Z_Q^{(1)}}$	χ^2/d.o.f.	θ_{zero}
1.50	120	111(5)	0.285(9)	0.90	3.00(12)
1.60	180	94(5)	0.325(6)	0.45	3.15(10)
1.70	340	67(3)	0.380(6)	1.04	3.11(9)
1.75	470	56(3)	0.412(5)	0.68	3.08(9)


0.3
0.2
0.1
0
1/ξ
β=1.5
β=1.55
$Q^{(2)}$
π^2
-12
-6
0
6
12
θ^2

$$\frac{c_1 + c_2 \theta^2}{1 + c_3 \theta^2}$$

β	$\boldsymbol{L}$	$(\theta_{\text{zero}})^2$	$\boldsymbol{Z_Q^{(2)}}$	χ^2/d.o.f.	θ_{zero}
1.50	110	10.4(1.0)	1.0	1.72	3.22(16)
1.55	150	9.7(1.0)	1.0	0.73	3.11(16)

(Bhanot-David)



Conclusions

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

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

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

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