A new approach to the two-dimensional σ model with a topological charge

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Outline

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The action $S_{O(3)}(\beta_{O(3)}, \theta)$ of the 2−dimensional (2D) non-linear σ model with a $\theta-$ term in the continuum reads

$$S_{O(3)}(\beta_{O(3)}, \theta) = \frac{1}{2}\beta_{O(3)} \int d^2x \, [\partial_\mu \vec{\sigma}(x)]^2 - i\theta S_q \ ,$$

[A. M. Polyakov (1975); E. Brézin and J. Zinn-Justin (1976)]

being $\beta_{O(3)}$ the inverse of the coupling constant, θ a real parameter, $\vec{\sigma}(x)$ a 3−component unit vector and S_q the topological charge given by

$$S_q = \frac{1}{8\pi} \int d^2x \ \epsilon^{\mu\nu} \epsilon^{kmp} \, \partial_\mu \sigma_k(x) \, \partial_\nu \sigma_m(x) \, \sigma_p(x) \ .$$

This model can be related with physical phenomena like, among others:

- in condensed-matter physics, superconductivity and quantum Hall effect;
  [E. Fradkin (1991)]
- in particle physics, asymptotic freedom, instantons and spontaneous generation of mass in non-Abelian gauge theories.

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Main features of the $\theta-$behavior of the model are the following:

- at $\theta = 0$, the spectrum exhibits a massive triplet of scalars;
  [P. Hasenfratz, M. Maggiore and F. Niedermayer (1990)]
- at $\theta = \pi$, the theory is massless (**Haldane conjecture**);
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- in the range $0 < \theta < \pi$, the spectrum develops a singlet (to be precise, it is already present at $\theta = \pi$) along with the triplet: their masses $m_S(\theta)$ and $m_T(\theta)$ are proportional to $(\pi - \theta)^{\frac{2}{3}}$ close to π.
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The above scenario has been verified - for the triplet - with different techniques trying to overcome the **sign problem** associated with the S_q term.
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Outline

1. Motivation
   - The model and the Haldane conjecture
2. The $SU(2)$ principal chiral model
   - First dual formulation
   - Second dual formulation
3. Preliminary results
   - Checks
   - First computations
4. Conclusions
   - Open issues and prospects

The strategy consists of relating the partition function $Z_{O(3)}(\beta_{O(3)}, \theta)$ of the original theory with the lattice partition function $Z_{SU(2)}(\beta)$ of the 2D $SU(2)$ principal chiral model reading

$$Z_{SU(2)}(\beta) = \int \prod_n DU(n) \exp\left(\beta \sum_{n'} \sum_{\mu=1}^{2} \mathrm{Tr}[U(n')U^\dagger(n' + \vec{e}_\mu)]\right) \ ,$$

where β is the (dual) counterpart of $\beta_{O(3)}$, $U(n) \in SU(2)$ and $n = (n_1, n_2)$ with $n_1, n_2 \in \{1, \ldots, L\}$. **Periodic boundary conditions will be assumed for the rest of this presentation.**

$Z_{SU(2)}(\beta)$ can be conveniently rewritten by introducing the link and plaquette variables $V(n,\mu)$ and $V(n)$ defined as

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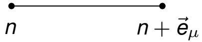

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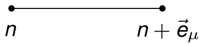

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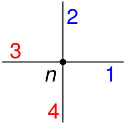

The $SU(2)$ matrix $V(n)$ can be parametrized as

$$V(n) = \exp[i\lambda_k \omega_k(n)] \ ,$$

with $[\lambda_k, \lambda_m] = 2i\epsilon^{kmp}\lambda_p$ and $\mathrm{Tr}[\lambda_k \lambda_m] = 2\delta_{km}$.

With this definitions, the partition function $Z_{SU(2)}(\beta)$ becomes

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where the index r labels the representation, $d(r)$ stands for the dimension of the representation r and $\chi_r[V(n)]$ is the character of $V(n)$ in the representation r.

For future convenience, let's introduce also the unconstrained $SU(2)$ model defined as

$$Z(\beta, R) = \int \prod_{(n,\mu)} dV(n,\mu) \exp\left[\beta \sum_{(n,\mu)} \mathrm{Tr}\, V(n,\mu)\right] \prod_{n'} \frac{\sin R\omega(n')}{\sin \omega(n')} \ .$$

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The continuum limit of the lattice $SU(2)$ principal chiral limit stems from the fact that, in the limit $\beta \to +\infty$, all link matrices perform small fluctuations around the identity.

[J. Bricmont and J.-R. Fontaine (1981)]

This allows replacing the $SU(2)$ $\delta-$function with the Dirac $\delta-$function, i.e.,

$$\sum_r d(r)\chi_r[V(n)] \longrightarrow \prod_{k=1}^{3} \int_{-\infty}^{\infty} e^{i\alpha_k(n)\omega_k(n)}\, d\alpha_k(n) \,,$$

and the continuum limit is achieved thanks to the following 3-step procedure:

- introduce dimensionful vector potentials $A_k(n)$ as $\omega_k(n) = aA_k(n)$ and expand in powers of the lattice spacing a;
- replace the $SU(2)$ invariant measure by a flat measure and extend the integration region over potentials $A_k(n)$ to the non-compact region $A_k(n) \in [-\infty, \infty]$;
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After neglecting terms vanishing in the limit $a \to 0$ and integrating over $A_k(n)$, the partition function $Z_{SU(2)}(\beta)$ eventually reads in the continuum

$$Z_{SU(2)}(\beta) \;=\; \int_{-\infty}^{\infty} \prod_{k=1}^{3} d\alpha_k(x)\; e^{-S_{\rm eff}(\beta)} \;,$$

with

$$S_{\rm eff}(\beta) = \frac{1}{4}\int d^2x\; \partial_\mu\alpha_k(x)\; M^{km}_{\mu\nu}(x)\; \partial_\nu\alpha_m(x) - \frac{1}{2}\int d^2x\; \ln[{\rm Det}\, M(x)] \;,$$

where

$$M^{km}_{\mu\nu}(x) = \frac{1}{\beta^2+\alpha^2(x)}\left[\delta_{\mu\nu}\left(\beta\delta_{km}+\frac{1}{\beta}\alpha_k(x)\alpha_m(x)\right) + i\,\epsilon^{\mu\nu}\,\epsilon^{kmp}\alpha_p(x)\right] \;,$$

being $\alpha^2(x) = \sum_{k=1}^{3}\alpha_k^2(x)$ and $Det\, M(x) = \beta^{-2}[\beta^2+\alpha^2(x)]^{-2}$.

Finally, another change of variables reading

$$\alpha_k(x) = R(x)\,\sigma_k(x) \qquad \left(\sum_{k=1}^{3} \sigma_k^2(x) = 1\right) ,$$

completes the computation of the continuum limit of $Z_{SU(2)}(\beta)$: it entails an integration over $R(x)$ and $\sigma_k(x)$.

However, it is much interesting to fix $R(x)$ to a constant value R: besides leading to the $a \to 0$ limit of the unconstrained $SU(2)$ principal chiral model, this choice allows for relating the latter to the non-linear σ model with a $\theta-$term since **in the continuum**

$$Z_{O(3)}(\beta_{O(3)}, \theta) = [C(\beta, R)]^{L^2}\, Z(\beta, R) ,$$

with

$$C(\beta, R) = \frac{\beta}{R}\left(R^2 + \beta^2\right) e^{-2\beta} .$$

The relations between the parameters are given by

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Thus, the procedure to numerically determine a given observable $\mathcal{O}(\sigma)$ of the non-linear σ model is well known:

- "translate" $\mathcal{O}(\sigma)$ into its counterpart $\tilde{\mathcal{O}}(V)$ with respect to the degrees of freedom of the $SU(2)$ unconstrained principal chiral model;
- tune (β, R) so to keep β large but in such a way that they correspond to the desired values of $(\beta_{O(3)}, \theta)$;
- measure $\tilde{\mathcal{O}}(V)$ by means of importance sampling and convert back to $\mathcal{O}(\sigma)$.

The algorithm employed in this study is a standard local Metropolis: since the probability distribution in $Z(\beta, R)$ is not necessarily positive due to the sine functions, a change leading to a configuration with negative weight is automatically dismissed.

This approach entails a bias that, however, "goes in the right direction" since, in the $\beta \to +\infty$ limit, such configurations are exponentially suppressed.

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Outline

In order to get some unbiased results to compare with, an alternative formulation for the unconstrained $SU(2)$ principal chiral model has been worked out.

Let's go back to $Z_{SU(2)}(\beta)$

$$Z_{SU(2)}(\beta) \;=\; \int \prod_{(n,\mu)} dV(n,\mu)\, \exp\left[\beta \sum_{(n,\mu)} \mathrm{Tr}\, V(n,\mu)\right] \prod_{n'} \left(\sum_r d(r) \chi_r[V(n')] \right) \;,$$

and let's assume a given representation r has been chosen for all $SU(2)$ matrices so that the partition function $\tilde{Z}(\beta, R)$ - with $R = 2r + 1$ - defined as

$$\tilde{Z}(\beta, R) = \int \prod_{(n,\mu)} dV(n,\mu)\, \exp\left[\beta \sum_{(n,\mu)} \mathrm{Tr}\, V(n,\mu)\right] \prod_{n'} \chi_r[V(n')] \;,$$

can be introduced.

It can be shown that

$$Z(\beta, R) \;=\; \tilde{Z}(\beta, R) \;,$$

when R appearing on the l.h.s. is **integer**.

In order to get some unbiased results to compare with, an alternative formulation for the unconstrained $SU(2)$ principal chiral model has been worked out.

Let's go back to $Z_{SU(2)}(\beta)$

$$Z_{SU(2)}(\beta) \;=\; \int \prod_{(n,\mu)} dV(n,\mu) \; \exp\left[\beta \sum_{(n,\mu)} \mathrm{Tr}\, V(n,\mu)\right] \prod_{n'} \left(\sum_r d(r) \chi_r[V(n')] \right) \;,$$

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can be introduced.

It can be shown that

$$Z(\beta, R) \;=\; \tilde{Z}(\beta, R) \;,$$

when R appearing on the l.h.s. is **integer**.

By definition, the character $\chi_r[V(n)]$ reads

$$\chi_r[V(n)] = \tilde{\sum}_n V(n,1)_{m_1 m_2} V(n,2)_{m_2 m_3} V^\dagger(n-\vec{e}_1,1)_{m_3 m_4} V^\dagger(n-\vec{e}_2,2)_{m_4 m_1} \ ,$$

where

$$\tilde{\sum}_n \equiv \sum_{m_1=-r}^{r} \sum_{m_2=-r}^{r} \sum_{m_3=-r}^{r} \sum_{m_4=-r}^{r} \ .$$

Therefore, $\tilde{Z}(\beta, R)$ can be rewritten as

$$\tilde{Z}(\beta, R) = \prod_n \tilde{\sum}_n \prod_{(n',\mu)} Q_{m_1 m_2 p_1 p_2}(n', \mu, \beta) \ ,$$

with

$$Q_{m_1 m_2 p_1 p_2}(n', \mu, \beta) = \int dV(n', \mu) \, \mathrm{e}^{\beta \, TrV(n',\mu)} V(n', \mu)_{m_1 m_2} V^\dagger(n', \mu)_{p_1 p_2} \ .$$

Dropping the dependence on (n, μ), the latter quantity becomes

$$Q_{m_1 m_2 p_1 p_2}(\beta) = \frac{1}{2r+1} \sum_{J}^{2r} \sum_{k=-J}^{J} C_J(\beta) C^{rp_2}_{rm_1,Jk}\, C^{rp_1}_{rm_2,Jk} \, ,$$

where $C^{rp_2}_{rm_1,Jk}$ are Clebsch-Gordan coefficients and

$$C_J(\beta) \;=\; \frac{2J+1}{\beta} I_{2J+1}(2\beta) \, .$$

being $I_{2J+1}(2\beta)$ Bessel functions.

Since

$$\sum_k C^{rp_2}_{rm_1,Jk} C^{rp_1}_{rm_2,Jk} = C^{rp_2}_{rm_1,J(p_2-m_1)} C^{rp_1}_{rm_2,J(p_1-m_2)} \delta_{p_2-m_1,p_1-m_2} \, ,$$

just 2 of the 4 magnetic numbers associated to each link are eventually free and the count of d.o.f. is restored.

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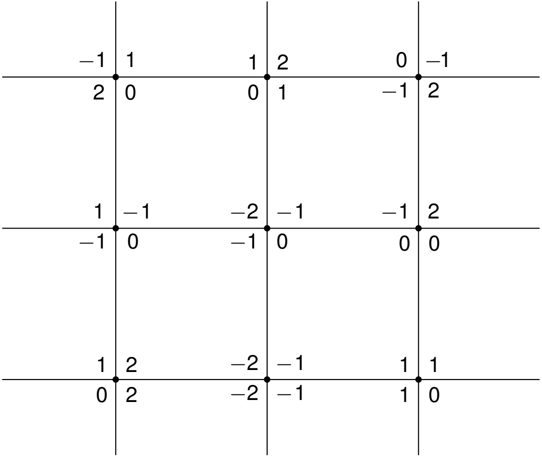
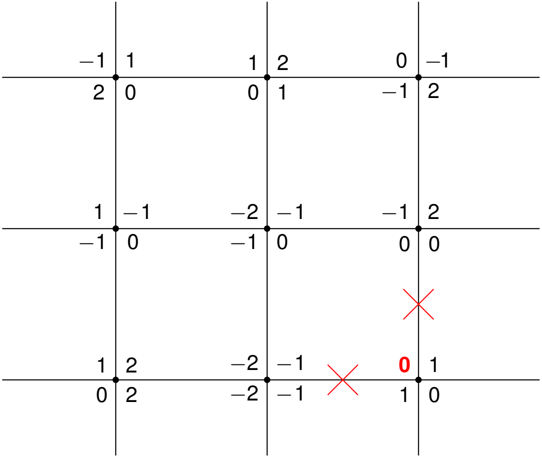
An example of allowed configuration with $R = 5$ (i.e., $r = 2$) with $L = 3$ is given by



A new configuration - to be submitted to a Metropolis test - is generated by introducing a discontinuity and by propagating it randomly till it is reabsorbed. For example,



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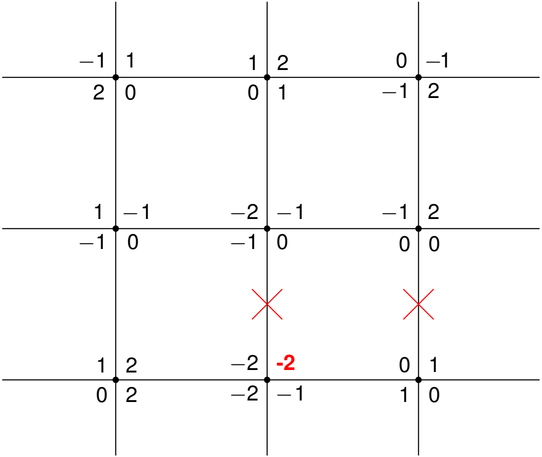

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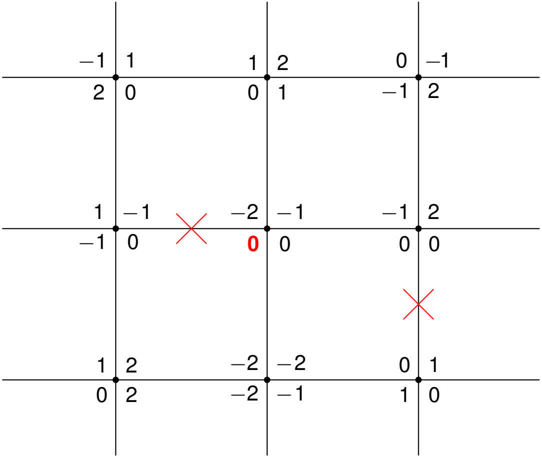

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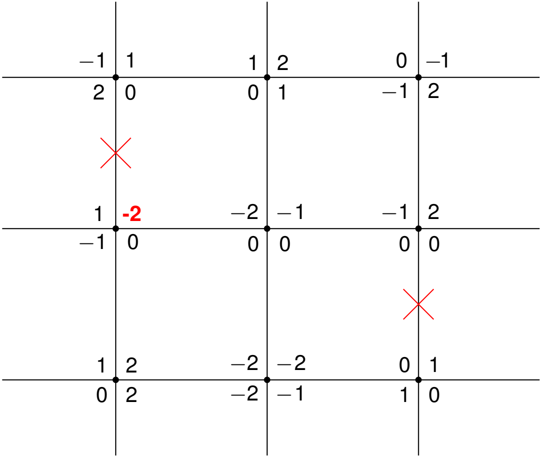

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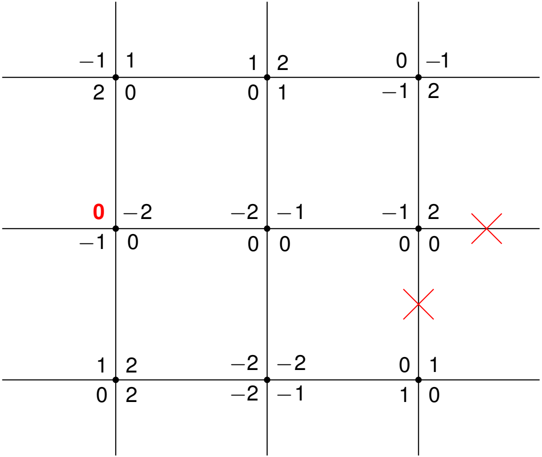

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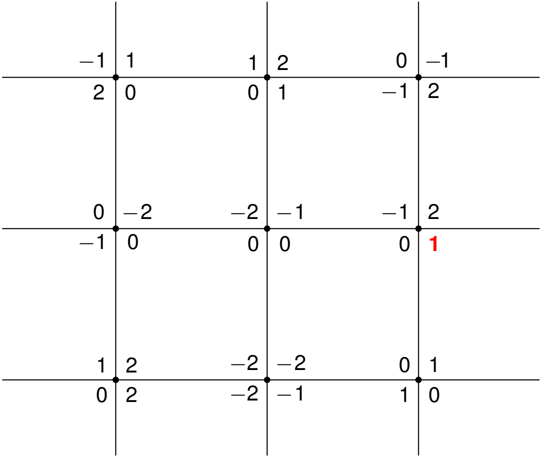

Outline

1. Motivation
   - The model and the Haldane conjecture
2. The $SU(2)$ principal chiral model
   - First dual formulation
   - Second dual formulation
3. Preliminary results
   - Checks
   - First computations
4. Conclusions
   - Open issues and prospects

Before computing quantities like correlators, let's test whether the overall strategy works by measuring less effort-demanding observables.

With respect to this, let's consider the following relation

$$
\begin{aligned}
\left.\frac{\partial ln[Z_{O(3)}(\beta_{O(3)},\theta)]}{\partial\beta_{O(3)}}\right|_{\beta_{O(3)}=\beta^*} &= \frac{\partial ln[Z(\beta,R)]}{\partial\beta}\left.\frac{\partial\beta}{\partial\beta_{O(3)}}\right|_{\beta_{O(3)}=\beta^*} + \\
&+ \frac{\partial ln[Z(\beta,R)]}{\partial R}\left.\frac{\partial R}{\partial\beta_{O(3)}}\right|_{\beta_{O(3)}=\beta^*} = \\
&= \langle\mathcal{O}_1(\beta,R)\rangle\left.\frac{\partial\beta}{\partial\beta_{O(3)}}\right|_{\beta_{O(3)}=\beta^*} + \langle\mathcal{O}_2\rangle(\beta,R)\left.\frac{\partial R}{\partial\beta_{O(3)}}\right|_{\beta_{O(3)}=\beta^*} .
\end{aligned}
$$

A first check will be performed by comparing numerical estimates for $\langle\mathcal{O}_1(\beta,R)\rangle$ with analytical results available in perturbation theory when expanding in β.

Note that $\langle\mathcal{O}_1(\beta,R)\rangle$ and $\langle\mathcal{O}_2(\beta,R)\rangle$ have to be **periodic** since the l.h.s. of the previous equation is.

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Another observable - computed only within the second dual formulation - is given by

$$\mathcal{O}_3(\beta, J) = \langle \sum_{k=-J}^{J} C^{rp_2}_{rm_1,Jk} C^{rp_1}_{rm_2,Jk} \rangle \ ,$$

whose analytical perturbative value reads

$$\mathcal{O}_3(\beta, J) = \frac{1}{(2J+1)} \frac{I_{2J+1}(2\beta)}{I_1(2\beta)} + O(\beta^{2J+2}).$$

valid for $J = 1, 2, 3$.

Outline

For both formulations, numerical estimates for $\mathcal{O}_1(\beta, r)$ and $\mathcal{O}_3(\beta, J)$ well agree with the corresponding analytical perturbative computations.

Observable	*Analytical*	1^{st} *form.*	2^{nd} *form.*
$O_1(0.1, 7.0)$	0.09983	0.100(18)	0.0999(6)
$O_1(0.3, 11.0)$	0.29560	0.296(17)	0.2956(17)
$O_1(0.5, 15.0)$	0.48039	–	0.4804(26)
$O_1(0.7, 15.0)$	0.64918	0.649(16)	–
$O_3(0.3, 1.0)$	0.00498	–	0.0049(61)
$O_3(0.5, 1.0)$	0.01308	–	0.0131(60)

Table: Comparison between computer results and analytical perturbative values for $\mathcal{O}_1(\beta, r)$ and $\mathcal{O}_3(\beta, J)$ with $L = 40$.

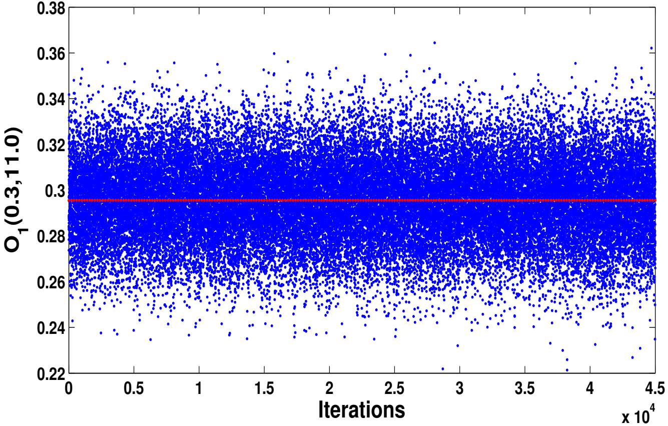

Figure: $O_1(\beta, R)$ vs. R with $\beta = 0.3$ and $R = 11.0$ ($L = 40$). The red line corresponds to the analytical result.

In the large-β regime, $O_1(\beta, R)$ qualitatively behaves as expected.

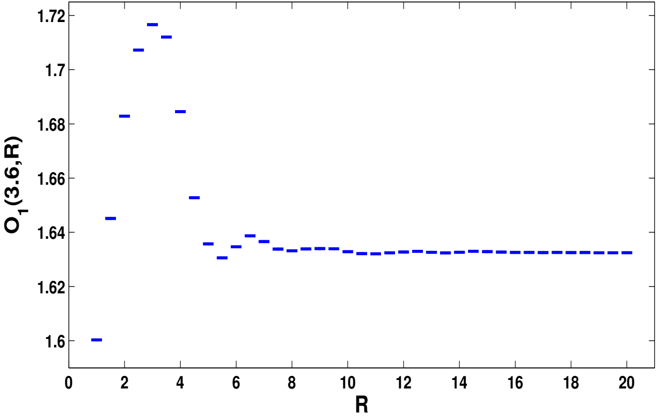

Figure: $O_1(\beta, R)$ vs. R at fixed $\beta = 3.6$ with $L = 200$.

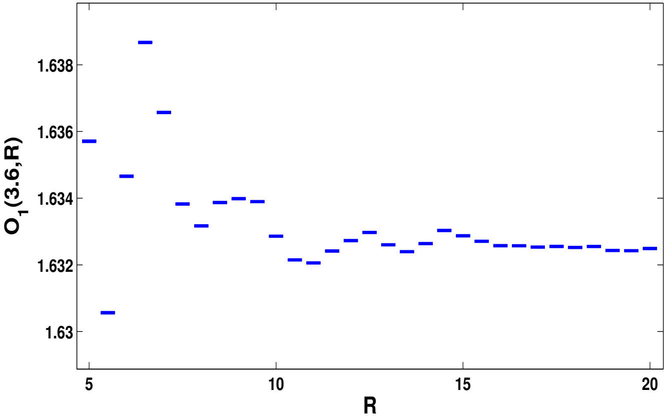

Figure: Blow-up of the previous figure in the large-R region.

However, when parameteres are fine-tuned, the desired periodic behaviour for $\mathcal{O}_1(\beta, R)$ is not observed.

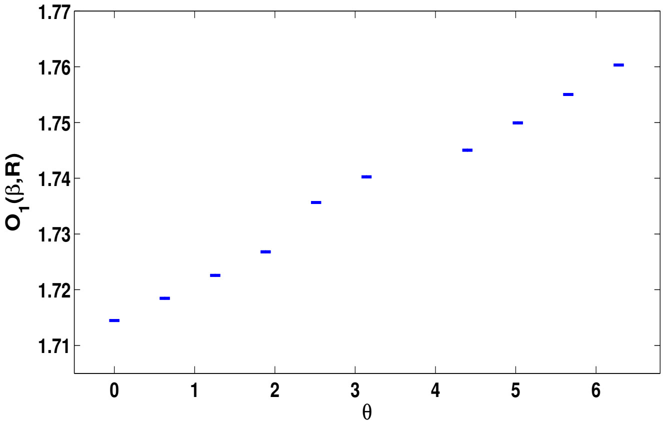

Figure: $\mathcal{O}_1(\beta, R)$ vs. θ: β ranges in $[4.5; 5.1]$ while R in $[6.56; 7.05]$ ($L = 200$).

Outline

To summarize:

- Two dual formulations for the non-linear σ model with a topological term have been introduced so to allow for numerical simulations with real θ
- computer results in the perturbative regime well agree with analytical computations
- however, the behaviour of the model at large β has still to be fully understood
- review of the theoretical aspects of the alternative formulations as well as of the numerical code has been undertaken

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The complete expression for $Z_{SU(2)}(\beta)$ in the continuum becomes

$$Z_{SU(2)}(\beta) = \int_0^\infty \prod_x \frac{R^2(x)dR(x)}{\beta\left(\beta^2+R^2(x)\right)} \int \prod_x \left[\delta\left(1-\sum_{k=1}^{3}\sigma_k^2(x)\right)\prod_{k=1}^{3} d\sigma_k(x)\right]$$
$$\times \exp\left[-\int d^2x\, \mathcal{L}[R(x),\sigma_k(x)]\right] ,$$

where

$$\mathcal{L}[R(x),\sigma_k(x)] \equiv \frac{1}{4}\,\partial_\mu[R(x)\sigma_k(x)]\, M^{km}_{\mu\nu}(x)\,\partial_\nu[R(x)\sigma_m(x)] ,$$

and

$$M^{km}_{\mu\nu}(x) = \frac{1}{\beta^2+R^2(x)}\left[\delta_{\mu\nu}\left(\beta\,\delta_{km}+\frac{R^2(x)}{\beta}\sigma_k(x)\,\sigma_m(x)\right)+i\,R(x)\,\epsilon^{\mu\nu}\,\epsilon^{kmp}\sigma_p(x)\right] .$$