Conjecture about the 2-Flavour QCD Phase Diagram

M A Nava Blanco\textsuperscript{1}, W Bietenholz\textsuperscript{2} and A Fernández Téllez\textsuperscript{1}

\textsuperscript{1} Facultad de Ciencias Físico Matemáticas, Benemérita Universidad Autónoma de Puebla, C.P. 72570 Puebla, Mexico

\textsuperscript{2} Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México, A.P. 70-543, C.P. 04510 Ciudad de México, Mexico

E-mail: miguelnava2539@gmail.com, wolbi@nucleares.unam.mx, afernan@mail.cern.ch

Abstract. The QCD phase diagram, in particular its sector of high baryon density, is one of the most prominent outstanding mysteries within the Standard Model of particle physics. We sketch a project how to arrive at a conjecture for the case of two massless quark flavours. The pattern of spontaneous chiral symmetry breaking is isomorphic to the spontaneous magnetisation in an O(4) non-linear $\sigma$-model, which can be employed as a low-energy effective theory to study the critical behaviour. We focus on the 3d O(4) model, where the configurations are divided into topological sectors, as in QCD. A topological winding with minimal Euclidean action is denoted as a skyrmion, and the topological charge corresponds to the QCD baryon number. This effective model can be simulated on a lattice with a powerful cluster algorithm, which should allow us to identify the features of the critical temperature, as we proceed from low to high baryon density. In this sense, this projected numerical study has the potential to provide us with a conjecture about the phase diagram of QCD with two massless quark flavours.

1. Scales in Quantum Chromodynamics

Quantum Chromodynamics (QCD) provides a successful description of the strong interaction between quarks and gluons. If we only deal with massless quarks, then the QCD Lagrangian does not involve any dimensional parameter, which implies scale invariance at the classical level. At the quantum level, however, an intrinsic scale $\Lambda_{\text{QCD}}$ emerges, which breaks this invariance. Recently a careful study derived, based on lattice simulations, the value $\Lambda_{\text{QCD}} = 341(12)\text{ MeV}$ (with $N_f = 3$ quark flavours, in the $\overline{\text{MS}}$-scheme) [1].

In the real world, the quarks do have masses, but two flavours are very light compared to the intrinsic scale. At 2 GeV, again in the $\overline{\text{MS}}$-scheme, their masses are [2]

$$m_u = 2.2^{+0.6}_{-0.4}\text{ MeV} , \quad m_d = 4.7^{+0.5}_{-0.4}\text{ MeV} , \quad m_u, m_d \ll \Lambda_{\text{QCD}} .$$

(1.1)

These two flavours dominate the low-energy nuclear physics, which matters for our daily life.\textsuperscript{1} It is therefore a sensible approximation to consider only two flavours, and — depending on the subject of interest — we may even neglect their masses.

\textsuperscript{1} Sometimes also the $s$-quark is considered as light, $m_s = 96^{+4}_{-3}\text{ MeV}$ [2]; in fact, it contributes to some low-energy quantities at the percent level. The remaining three quark flavours $c, b, t$ have masses well above $\Lambda_{\text{QCD}}$; they are usually negligible at low energy.
2. Chiral flavour symmetry breaking

If fermions are massless, their left- and right-handed components decouple. In the case of \( N_f \) massless quark flavours, each chirality can undergo an independent unitary transform, which corresponds to a global symmetry

\[
U(N_f)_L \otimes U(N_f)_R = SU(N_f)_L \otimes SU(N_f)_R \otimes U(1)_B \otimes U(1)_A
\]  
(2.1)

of the QCD Lagrangian. However, also part of this symmetry breaks explicitly due to quantum effects: in particular, the invariance under the group \( U(1)_A = U(1)_L = U(1)_R \) — which corresponds to opposite phase shifts for the left- and right-handed quarks — is broken by the axial anomaly [3]. The rotations with equal phases are captured by the symmetry group \( U(1)_B = U(1)_L = U(1)_R \), which corresponds to baryon number conservation.

The remaining chiral flavour symmetry breaks spontaneously,

\[
SU(N_f)_L \otimes SU(N_f)_R \rightarrow SU(N_f)_{L=R},
\]  
(2.2)

which gives rise to \( N_f^2 - 1 \) Nambu-Goldstone bosons (NGBs). For massive but light quarks they turn into light quasi-Nambu-Goldstone bosons, which are identified with the pion triplet (for \( N_f = 2 \)), or the octet of pions, kaons and the \( \eta \)-meson (for \( N_f = 3 \)).

Generally, NGB fields take their values in the coset space of the spontaneous symmetry breaking. Therefore, in the case of transition (2.2), we obtain NGB fields \( U(x) \in SU(N_f) \). Chiral perturbation theory formulates a low-energy effective theory in terms of NGB fields [4]; in this case, its leading order Lagrangian reads (in Euclidean space)

\[
\mathcal{L}(\partial_\mu U) = \frac{F_\pi^2}{4} \text{Tr} \left( \partial_\mu U \partial_\mu U^\dagger \right),
\]  
(2.3)

where \( F_\pi \simeq 92 \text{ MeV} \) is the pion decay constant. Higher order terms in this low-energy expansion involve at least four derivatives (in addition the quark masses can be incorporated).

At fixed Euclidean time \( x_4 \), the field \( U \) maps the 3d coordinate space to the group \( SU(N_f) \). The identity \( \Pi_3[SU(N_f)] = \mathbb{Z} \) implies that these maps are divided into topological sectors, labelled by a topological charge \( Q \in \mathbb{Z} \). In this case, it is given by the term

\[
Q = \frac{1}{24\pi^2} \int d^3x \epsilon_{ijk} \text{Tr} \left( (U \partial_i U)(U \partial_j U)(U \partial_k U) \right), \quad i, j, k \in \{1, 2, 3\},
\]  
(2.4)

which is conserved in time (so we are not really restricted to some instant \( x_4 \)). Amazingly, it can be interpreted as the baryon number, although the NGB fields apparently just represent mesons [5]; for a comprehensive review we refer to Ref. [6].

Actually the leading order Lagrangian (2.3) does not allow for a stable semi-classical solution with \( Q = 1 \). In order to stabilise such a skyrmion (a type of soliton), Skyrme added a four-derivative term [5], which can be written as [7]

\[
\mathcal{L}_{\text{Skyrme}}(U, \partial_\mu U) = \frac{F_\pi^2}{4} \text{Tr} \left( \partial_\mu U \partial_\mu U^\dagger \right) + \frac{1}{32e^2} \text{Tr} \left[ (\partial_\mu U)^\dagger (\partial_\mu U)^\dagger \right]^2,
\]  
(2.5)

where \( e \) is a dimensionless parameter. The skyrmion represents a fermionic (bosonic) baryon for an odd (even) number of colors, \( N_c \). The Skyrme model works reasonably well as an effective theory for QCD, with \( N_c = 3 \) and baryons included. Predictions for hadronic quantities like the nucleon and \( \Delta \) mass, \( F_\pi \), magnetic moments and charge radii were obtained within about 30% of the experimental values [7], although there is some tension of this higher-order term, and of the heavy skyrmion mass, with the low-energy assumption.
3. The 3d O(4) model as a low-energy effective theory

In view of the search for a simpler, effective theory, it is of interest to describe the symmetry breaking pattern (2.2) by (locally) isomorphic orthogonal groups, \( O(N) \rightarrow O(n), N > n \). This is possible solely for \( N_f = 2 \), where the transition (2.2) isomorphically corresponds to \( O(4) \rightarrow O(3) \).

Therefore the O(4) non-linear \( \sigma \)-model represents an effective theory for low-energy QCD with \( N_f = 2 \) massless quark flavours. Its Euclidean action

\[
S[\vec{e}'] = \frac{F^2}{2} \int d^4x \partial_\mu \vec{e}(x) \cdot \partial_\mu \vec{e}(x), \quad \vec{e}(x) \in S^3, \tag{3.1}
\]
corresponds to the QCD low-energy Lagrangian for \( N_f = 2 \) massless quark flavors. The global O(4) symmetry may break spontaneously down to O(3), which yields three NGBs, with fields in the coset space O(3), which is isomorphic to SU(2).

We focus on the O(4) model in 3-dimensional Euclidean space — the O(4) Heisenberg ferromagnet — as a static Skyrme model. In fact, the critical points — i.e. the second order phase transitions — in both models seem compatible [9]; for a review, which addresses this topic, we refer to Ref. [10]. The critical exponents of the 3d O(4) model were estimated some time ago (referring to the anti-ferromagnetic regime for agreement with the universality class of 2-flavour QCD) [11], and recently the scaling in the critical regime has been studied numerically [12, 13]. Precise numerical values of the critical temperature and critical exponents are summarised in Ref. [13], based on previous work [14].

However, these studies did not pay particular attention to the fact that in this model, the configurations are divided into topological sectors, as in the 4d Yang-Mills SU(\(N\)) gauge theories (\( N \geq 2 \)), and in QCD. Thus the skyrmions are also present in the 3d O(4) formulation of the low-energy effective theory, which therefore describes QCD at finite baryon density, although this link is not rigorous. No stabilising extra term is required in this static model.

4. Skyrmions on the lattice

The goal of this project is a study of the 3d O(4) model, considering in particular the rôle of the skyrmions as carriers of the baryon number. Since these are topological properties, such a study must be non-perturbative.

The only fully controlled non-perturbative approach to quantum field theory is based on Monte Carlo simulations of the lattice regularised system (for a recent review, see e.g. Ref. [15]). For the O(\(N\)) models, the Wolff cluster algorithm [16] turned out to be extremely efficient: it proceeds by updating entire spin clusters in a sophisticated manner. This is far superior to local update algorithms, which suffer, for instance, from an extremely long auto-correlation time with respect to the topological charge \( Q \) as one approaches the critical point ("topological freezing").

Strictly speaking, the standard lattice action

\[
S[\vec{e}'] = \frac{F^2}{2} \sum_{(xy)} (1 - \vec{e}_x \cdot \vec{e}_y), \quad \vec{e}_x \in S^3, \tag{4.1}
\]
(where the sum runs over all nearest neighbor lattice sites \( x, y \)) does not have topological sectors by default; all configurations can be continuously deformed into one another. Nevertheless, a variety of ways have been suggested to define a topological charge on the lattice; in particular the geometric definition has the virtue of guaranteeing integer charges, \( Q \in \mathbb{Z} \), for all configurations (except for a subset of measure zero). It was suggested and successfully applied in the 2d O(3) model\(^3\) [17], where the lattice plaquettes are split into triangles, and the topological charge

\(^2\) The inclusion of quark masses corresponds here to the addition of an external "magnetic field" \( \vec{H} \), i.e. a term \(-\vec{H} \cdot \vec{e}(x)\) in the Lagrangian, which explicitly breaks the O(4) symmetry.

\(^3\) Generally, the O(\(N+1\)) model has topological sectors in \( N \) dimensions, due to \( \Pi_N[S^N] = \mathbb{Z} \).
density is given by the (minimal) oriented area of the spherical triangle spanned by the spins at its vertices.

In addition to its efficiency, the cluster algorithm enables a dynamical definition of merons [18] (objects of half-integer topological charge). Their properties were explored in the 2d O(3) model [18] and in the 1d O(2) model (the quantum rotor) [19]. It is straightforward to apply the same concept to the 3d O(4) model.4

In order to extend the (sound) geometric definition of $Q$ to the 3d O(4) model, we decompose all lattice unit cubes into five tetrahedra, as illustrated in Figure 1, as described for instance in Ref. [20] (four of them are congruent, while only the fifth one is regular).5 For a given

![Figure 1](image.png)

**Figure 1.** Illustration of the division of a lattice unit cube into five tetrahedra. This leads to space-filling set of tetrahedra. The spins at its vertices span spherical tetrahedra on $S^3$, and their oriented volumes represent the lattice topological charge density.

tetrahedron, the spin variables $\vec{e}_x$, $\vec{e}_y$, $\vec{e}_z$, $\vec{e}_w$ at the four vertices span a *spherical tetrahedron* on the 3-dimensional sphere $S^3$. Its volume can be computed according to the formulae elaborated only recently in Refs. [21]. We can assign a sign to each spherical tetrahedron according to its orientation, by invoking the sign of $\det(\vec{e}_x, \vec{e}_y, \vec{e}_z, \vec{e}_w)$.

For a given lattice configuration in some volume $V$ with periodic boundary conditions, lattice unit cubes are split into tetrahedra, and all volumes of the corresponding oriented spherical tetrahedra are summed up to obtain the topological charge $Q \in \mathbb{Z}$ — it counts how many times the sum of the spherical tetrahedra covers the sphere $S^3$.

With the basic action (4.1) its expectation value vanishes, $\langle Q \rangle = 0$, due to parity symmetry. This symmetry can be broken, however, by adding a chemical potential. In this formulation it couples directly to the topological charge, without causing a sign problem. Alternatively, an isospin chemical potential has been included in the Skyrme model with the usual prescription of a covariant derivative in the Euclidean time direction [22].

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4 Moreover, in Refs. [18, 19] the meron cluster algorithm gave rise to an improved estimator as a very powerful numerical tool. However, its application to the 3d O(4) model requires rather restrictive constraints on the relative angles between neighbouring spins. This enforces a limitation to smooth configurations, which may obstruct the observation of the phase transition, hence we dispense with this technique in the ongoing study.

5 In the 2d O(3) model, an alternative is the use of a lattice consisting of equilateral triangles [18]. The analogue recipe fails, however, in $d = 3$, since regular tetrahedra are not space-filling (contrary to a claim by Aristotle, which caused long-term confusion [20]).
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