Quantum Phase Transitions within a nuclear cluster model and an effective model of QCD

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Abstract

The catastrophe theory is applied to a nuclear cluster model and an effective model for QCD at low energy. The study of quantum phase transitions in the cluster model was considered in an earlier publication, but restricted to spherical clusters and on a semi-classical level. In the present contribution, we include the case of deformed clusters and determine the spectrum numerically as a function of an interaction parameter, where signatures of a quantum phase transition can be seen. It is shown that in this more complicated case, with deformation of the clusters, the catastrophe theory can be applied with some interesting consequences. A further example of a many-body problem is considered, namely an effective model of QCD, which is able to describe the low energy hadron spectrum and, when temperature is introduced, even ratios of particle-antiparticle productions. The catastrophe theory is able to provide useful information on the phase transition from a perturbative to a non-perturbative vacuum. This contribution shows the universal usefulness of catastrophe theory, while more examples of applications to different fields are mentioned in the Introduction.

Keywords: quantum phase transitions, cluster model, algebraic model

1. Introduction

In a recent contribution, we applied the catastrophe theory to the Semimicroscopic Algebraic Cluster Model (SACM), in order to describe Quantum Phase Transitions (QPTs). The SACM was chosen because it exhibits quite complex semi-classical potentials and, therefore, serves as a test-bed for the applied method and how to proceed in more complex models. In the study of QPTs was limited to spherical clusters on a semi-classical level. In this contribution we include deformed clusters, which introduces a higher complexity in the semi-classical analysis. In addition, explicit numerical diagonalisations of the Hamiltonian are done and the spectrum is retrieved as function of an interaction parameter, which will show characteristics related to the phase transitions.

Another motivation of this contribution is to show the effectiveness of the catastrophe theory and its wide range of applications to quite different fields in physics, all related to many-particle
physics but from a different perspective. We will apply it to an effective model of QCD at low energy. First steps into this direction were presented in [3, 4, 5, 6], using standard methods. With the catastrophe theory we can deduce the order of the phase transition and describe important changes in the structure of the vacuum state of QCD.

There are applications even to General Relativity. For example, in [7] the catastrophe theory was applied to a rotating black hole, with a Kerr metric. Phase transitions were related to the appearing and disappearing of the event-horizon of black holes and to the positions of light rings. A further application can be found in Optics and we refer to the book [8].

The paper is structured as follows: In Section 2 we discuss the extension of the SACM to include deformation of the clusters and the obtention of the semi-classical potential. Two examples are considered, one of spherical clusters and one of deformed clusters, and the study of QPTs, semi-classically and numerically, is done. In Section 3 the catastrophe theory will be applied to an effective model of QCD at low energy and the many-body structure of the vacuum state is investigated. In Section 4 Conclusions will be drawn.

2. QPTs within the SACM and their signatures

Cluster models play an important role in nuclear physics. There are two main groups of cluster models: The microscopic cluster models, which can be represented by [9], and algebraic cluster models. The last group can be divided into the ones which do not satisfy the Pauli Exclusion Principle (PEP), for example [10], and those which do observe the PEP, for example the SACM [11, 12]. The importance of satisfying the PEP and the consequences of the PEP not being observed can be found in [13, 14]. There is another important line of models able to study the clusterization of nuclei, namely [15, 16, 17], which uses a Symmetry Adapted basis in reducing the shell model space. The cluster structure is investigated via overlaps of a symplectic basis with cluster wave functions.

Phase transitions in algebraic models were discussed in [18], for the IBA [19], and in various other algebraic models in [20, 21, 22, 23]. In particular, in [24] the catastrophe theory was applied to these algebraic models. Here, we will apply it to the SACM [11, 12]. For completeness, a short summary is presented on the algebraic cluster model considered.

The SACM was proposed in 1994 [11, 12] and differs from most algebraic clusters models because it takes into account the PEP. The relative motion of the clusters is described by the generators of the $U_R(4)$ group, which are the 16 combinations of the creation ($\pi^+_m,\sigma^+$) and annihilation ($\pi^m,\sigma$) operators of the $\pi$ bosons (with angular momentum $\ell = 1$) and the $\sigma$ bosons (with angular momentum $\ell = 0$): $\pi^+_m,\pi^+_m,\sigma,\sigma^+\pi^m,\sigma^+\sigma$.

The Pauli exclusion principle is considered in the way on how the space of the SACM is constructed. Each cluster is described by an $(\lambda_k,\mu_k)$ irreducible representation (irrep) within the SU(3) shell model, while the relative motion is also described as an $(n_{\pi},0)$ irrep, with the PEP being accounted for partially through the Wildermuth condition [25], which imposes a minimum value to the number of $\pi$ bosons: $n_{\pi} \geq n_0$. Then, the space is constructed as the direct product of these irreps,

$$(\lambda_1,\mu_1) \otimes (\lambda_2,\mu_2) \otimes (n_{\pi},0) = \sum_{(\lambda,\mu)} m_{\lambda,\mu}(\lambda,\mu),$$

(1)
where $m_{\lambda,\mu}$ is a multiplicity factor. The resulting sum of irreps is finally compared with the space of the SU(3) shell model of the nucleus considered and only those irreps are maintained which appear in the shell model. In such a manner, the PEP is accounted for.

The *semi* prefix in the name of the model is because the Hamiltonian operator is phenomenological and is composed of Casimir operators of the dynamical symmetries. For the relative motion, there are two group chains of U(4) which contains the group SO(3) of angular momentum:

$$U(4) \supset SU(3) \supset SO(3) \supset SO(2)$$

$$U(4) \supset SO(4) \supset SO(3) \supset SO(2)$$ \hspace{1cm} (2)

defining the dynamical symmetry (here we omitted the $R$ subscript of the relative motion). As an example we consider a simplified (not the most general) Hamiltonian operator, consisting of linear combinations of Casimir operators of the groups SU(3) and SO(4) up to second order:

$$H = H_{SU(3)} + H_{SO(4)}$$ \hspace{1cm} (3)

with

$$H_{SU(3)} = \hbar \omega \pi + (\bar{a} - \bar{b} \Delta \pi) C_2(\pi, 0) + (a - b \Delta \pi) C_2(\lambda, \mu) + \xi L^2 + t_1 K^2$$ \hspace{1cm} (4)

$$H_{SO(4)} = \frac{c}{4} [(\pi^\dagger \cdot \pi^\dagger) - (\sigma^\dagger)^2] [(\pi \cdot \pi) - (\sigma)^2],$$ \hspace{1cm} (5)

with $\Delta \pi = \pi - n_0$, and $n_0$ is the minimal number of relative oscillation quanta determined by the Wildermuth condition \[25\]. The $\hbar \omega$ is given by $45A^{-\frac{1}{2}} - 25A^{-\frac{3}{2}}$ \[26\] and, thus, is fixed. The Hamiltonian depends on 7 parameters $\{a, b, \bar{a}, \bar{b}, c, \xi, t_1\}$, all in units of MeV. The operator $K^2$ is introduced to address the degeneracy of excited states. The eigenvalues of the second order Casimir, the angular momentum and $K^2$ operators are

$$C_2(\lambda, \mu) \rightarrow \lambda^2 + \lambda \mu + \mu^2 + 3\lambda + 3\mu$$

$$L^2 \rightarrow L(L+1)$$

$$K^2 \rightarrow K^2$$ \hspace{1cm} (6)

where $K$ is the quantum number labelling the rotational bands.

After having set up the model Hamiltonian, the next step is to define the semi-classical potential. As this was already done in \[1\], we restrict to a short summary, adding the contributions due to the deformation of the clusters.

The semi-classical potential is obtained as the expectation value of the Hamiltonian operator in the basis of the coherent states of the SACM, which are defined as \[27\]

$$|\alpha\rangle = \frac{N!}{(N + n_0)!} N_{N,n_0} \frac{d^{n_0}}{d\gamma_{n_0}} [\sigma^\dagger + \gamma (\alpha^\ast \cdot \pi^\dagger)]|0\rangle \bigg|_{\gamma=1} \hspace{1cm} (7)$$

where

$$N_{N,n_0}^{-2} = \frac{(N!)^2}{(N + n_0)!} \frac{d^{n_0}}{d\gamma_{1,n_0}} \frac{d^{n_0}}{d\gamma_{2,n_0}} [1 + \gamma_1 \gamma_2 (\alpha^\ast \cdot \alpha)]^{N+n_0} \bigg|_{\gamma_1=\gamma_2=1}. \hspace{1cm} (8)$$
\(N_{N,n_0}^{-2}\) is the normalization constant and \(\alpha_m\) are arbitrarily complex variables. We consider the simple case in which \(\alpha_m\) transforms as a tensor, as was previously done in [28], and choose the parametrization \(\alpha_{\pm 1} = \alpha_{-1} = 0\) and \(\alpha_0 = i\alpha\), where the variable \(\alpha\) can be related to the distance between the clusters [27].

The semi-classical potential results in a function of one variable \(\alpha\):

\[
V(\alpha; c_i) = \langle \alpha | H | \alpha \rangle = V_0 - (b + \bar{b}) \left( A \alpha^2 \frac{F_{11}(\alpha)}{F_{00}(\alpha)} + B \alpha^4 \frac{F_{22}(\alpha)}{F_{00}(\alpha)} + C \alpha^2 \frac{F_{20}(\alpha)}{F_{00}(\alpha)} \right),
\]

with the constant value \(V_0\) given by

\[
V_0 = (a + n_0 b) \langle C_2(\lambda_C, \mu_C) \rangle + \xi \langle L_2^2 \rangle + \frac{c}{4} (N + n_0)(N + n_0 - 1),
\]

where \((\lambda_C, \mu_C)\) is an intermediate irrep of the cluster system given by the product \((\lambda_1, \mu_1) \otimes (\lambda_2, \mu_2)\) in [11].

The 3 control parameters \(c_i = \{A, B, C\}\) are linear combinations of the Hamiltonian parameters:

\[
A = -\frac{1}{b + \bar{b}} \left[ \hbar \omega - b \langle C_2(\lambda_C, \mu_C) \rangle + 4(a + \bar{a} + (b + \bar{b})(n_0 - 1)) + (a + b(n_0 - 1))(\Gamma_1 + \Gamma_2) + 2 \xi - \frac{c}{2} (N + n_0 - 1) \right]
\]

\[
B = -\frac{1}{b + \bar{b}} \left[ a + \bar{a} + (b + \bar{b})(n_0 - 6) - b(\Gamma_1 + \Gamma_2) + \frac{c}{2} \right]
\]

\[
C = \frac{1}{b + \bar{b}} c .
\]

The deformation of the clusters is taken into account via the \(\Gamma_k\), which is the expectation value of the \(m = 0\) component of the quadrupole operator of cluster \(k\) [28]:

\[
\Gamma_k = \langle (\lambda_k, \mu_k) | Q_0^C_k | (\lambda_k, \mu_k) \rangle = \sqrt{\frac{5}{\pi}} \left( n_k + \frac{3}{2} (A_k - 1) \right) \beta_k .
\]

The \(n_k\) is the total number of quanta of the deformed cluster and \(\beta_k\) is the quadrupole deformation. The \(F_{pq}(\alpha^2)\) functions in [9] are defined in [28]:

\[
F_{pq}(\alpha^2) = \frac{(N!)^2}{(N + n_0 - \max(p, q))!} \times \sum_{k=\max(n_0-p,n_0-q)}^{N+n_0-\max(p,q)} \binom{N + n_0 - \max(p, q)}{k} \frac{(k + p)!}{(k + p - n_0)!} \frac{(k + q)!}{(k + q - n_0)!} \alpha^{2k} .
\]

2.1. Catastrophe theory and the parameter space

A useful and systematic way of determining how the change of parameters affects a function’s critical points is with the help of catastrophe theory [2]. For details, concerning the first application to the SACM, please consult [1].
The parameter space will be divided into regions of similar qualitative behaviour of the potential. Two separatrices, which divide regions of different behaviours, of importance are to be constructed: The bifurcation and the Maxwell sets.

- Bifurcation set: Is the subspace of parameter space delimiting the emergence of extreme values of the potential.
- Maxwell set: Is the subspace of parameter space where two or more extreme values of the potential are the same, i.e. for $\alpha_1$ and $\alpha_2$ critical points we have $V(\alpha_1) = V(\alpha_2)$.

In Appendix A a general expressions for the calculations of the bifurcation set and the Maxwell set, for an arbitrary potential function, are presented.

![Figure 1: Parameter space ($r_1, r_2$).](image)

Figure 1: Parameter space ($r_1, r_2$). The $r_2$-axis is drawn as a blue continuous line for $r_2 > 0$, where $\alpha = 0$ is a minimum point, and as a blue dashed line for $r_2 < 0$, where $\alpha = 0$ is a maximum point; in both cases the critical point has a fourth order multiplicity. The bifurcation set is drawn as a light blue line, and the Maxwell set as a red line. The light blue dashed line is the continuation of the bifurcation set, which is obtained by joining the end of the bifurcation set to the end of the Maxwell set. The stability separatrix in (21) is drawn as a purple line. The particular characteristics which define each region are described in the text.

A first step in the catastrophe theory formalism is the determination of the essential parameters [18], which are the minimum number of parameters necessary for a complete description
of the potential and are combinations of the original control parameters. They are obtained by expanding the potential in a Taylor series about the fundamental root. We may identify the origin $\alpha = 0$ as the fundamental root since it is always a critical point of the semi-classical potential (9) for all values of the control parameters. Then, by choosing combinations of the control parameters such that the first terms in the Taylor series vanish, until it is no longer possible to eliminate the next term, which is called the germ of the potential, we determine the essential parameters.

A Taylor series expansion of the semi-classical potential (9) about $\alpha = 0$ yields:

$$V(\alpha; c_i) = V_0 - (b + \bar{b})(T_0 + T_1 \alpha^2 + T_2 \alpha^4 + \ldots ),$$

(14)

and the first $T_i$ coefficients are given by

$$T_0 = n_0 A + n_0 (n_0 - 1) B + n_0 (n_0 - 1) (n_0 - 2)$$

$$T_1 = N (n_0 + 1) A + 2 N (n_0 + 1) n_0 B + 3 N (n_0 + 1) n_0 (n_0 - 1)$$

$$+ \frac{1}{2} N (N - 1) (n_0 + 2) (n_0 + 1) C$$

$$T_2 = N (n_0 + 1) \left( N - (n_0 + 2) \right) A + N (n_0 + 1) \left( 2 (N - 1) - n_0 (2 n_0 + 5 - 3 N) \right) B$$

$$+ 3 N (n_0 + 1) n_0 \left( N (2 n_0 + 1) - 2 n_0 (n_0 + 1) \right)$$

$$+ \frac{1}{3} N (N - 1) (n_0 + 2) (n_0 + 1) \left( n_0 (N + 1) + 3 \right) C.$$

(15)

The semi-classical potential is then redefined as

$$\bar{V}(\alpha; c_i) = V(\alpha; c_i) - V_0 + (b + \bar{b}) T_0,$$

(16)

so that we have $\bar{V}(\alpha \to 0; c_i) = 0$. By straightforward algebraic manipulation of the $F_{pq}(\alpha)$ functions we are able to write the semi-classical potential as:

$$\bar{V}(\alpha, r_i) = \frac{r_3}{Q_0(\alpha)} \left[ r_1 Q_1(\alpha) + r_2 Q_2(\alpha) + Q_3(\alpha) + r_4 Q_4(\alpha) \right],$$

(17)

with the essential parameters $r_i$ defined by

$$r_1 = A + 2 n_0 B + 3 n_0 (n_0 - 1) + \frac{1}{2} (N - 1) (n_0 + 2) C$$

$$r_2 = B + 3 n_0 - \frac{1}{6} (n_0 (N + 1) + 6) C$$

$$r_3 = -(b + \bar{b})$$

$$r_4 = \frac{1}{6} n_0 (N + 1) C,$$

(18)

and define the $Q_i(\alpha)$ polynomials by

$$Q_i(\alpha) = \sum_{k=i}^{N} \frac{N!}{(N-k)!} \frac{(n_0+k)!}{n_0!} \frac{\alpha^{2k}}{k!(k-i)!}$$
\[ Q_4(\alpha) = \sum_{k=3}^{N} \frac{N!}{(N-k)!} \frac{(n_0 + k)!}{n_0!} \frac{\alpha^{2k}}{(k+1)!(k-3)!}, \]  

(19)

with \( i = 1, 2, 3 \). In (16) and (18) we can see that from \( T_1 = 0 \) we obtain \( r_1 \), and similarly from \( T_2 = 0 \) we get \( r_2 \); lastly, \( r_3 \) and \( r_4 \) are the leftover parameters. The next term of the Taylor series \( T_3 \) can no longer be eliminated, thus identifying the germ of the potential as \( \alpha^6 \).

The stability of the potential is determined through the limits \( \alpha \to \infty \) and \( N \to \infty \). A potential is stable if in the limit \( \alpha \to \infty \) it tends to a positive value, otherwise, if it tends to a negative value the potential is unstable (the system disintegrates when approaching infinity). Using the expressions in (19) we readily obtain the limit \( \alpha \to \infty \) of the semi-classical potential (17):

\[ \lim_{\alpha \to \infty} V(\alpha; r_i) = r_3 N \left( r_1 + r_2 (N-1) + (N-1)(N-2) + r_4 \frac{(N-1)(N-2)}{N+1} \right), \]  

(20)

and the global \( N \) indicates that in the limit \( N \to \infty \) the potential will either tend to plus (stable) or minus (unstable) infinity. By demanding (20) to be zero we obtain the separatrix in parameter space

\[ r_1 + r_2 (N-1) + (N-1)(N-2) + r_4 \frac{(N-1)(N-2)}{N+1} = 0, \]  

(21)

which divides the parameter space in regions of stable and unstable potentials.

In the following sections we will study the quantum phase transitions of two separate cases:

- The limit SU(3) of the Hamiltonian (3), i.e. \( c = 0 \), when the essential parameter space is two-dimensional \((r_1, r_2)\). This part is mostly a repetition of [1]. However, it contains some new elements: A series of paths for two example systems in the parameter space and their effects as avoided level crossing of states as a function of \( \bar{a} \) are considered.

- The Hamiltonian (3) has a mixture of SU(3) and SO(4) symmetries, i.e. \( c \neq 0 \) and the essential parameter space is three-dimensional \((r_1, r_2, r_4)\).

2.2. QPTs in the SU(3) limit: \( c = 0 \)

For this case, two example systems will be considered: The system \(^{16}\text{O} + \alpha \to ^{20}\text{Ne}\) of spherical clusters, and the system \(^{12}\text{C} + ^{12}\text{C} \to ^{24}\text{Mg}\) of deformed clusters. For each case the separatrices in the two-dimensional \((r_1, r_2)\) parameter space are constructed and QPTs are studied as one moves across different regions. The \(^{20}\text{Ne}\) clusterisation was considered in [1], while the \(^{24}\text{Mg}\) system is new, containing two well deformed cluster, i.e., we can study the effects of deformed clusters, not present in the first system. Another new ingredient is the numerical calculation of the spectrum, relating its structure to the appearance of phase transitions, as will be described by the semi-classical analysis. The software MATHEMATICA [29] was extensively used.
2.2.1. Spherical clusters example: $^{16}$O + $\alpha \to ^{20}$Ne

For this example we have $n_0 = 8$, deformations $\beta_{16}$O = 0, $\beta_{16}$a = 0, $(\lambda_1, \mu_1) = (\lambda_2, \mu_2) = (0, 0)$ and in the numerical diagonalisation of the Hamiltonian we will consider up to four excitation quanta, $N = 4$. With the values for $n_0$ and $N$ and direct application of the formulas in Appendix A we are able to construct the separatrices in parameter space $(r_1, r_2)$ depicted in Fig. 1. For regions I, II, III, IV and V the potentials tend to a positive value in the limit $\alpha \to \infty$: $V(\alpha \to \infty) > 0$; and for regions VI, VII, VIII and IX the potentials tend to a negative value in this limit $\alpha \to \infty$: $V(\alpha \to \infty) < 0$. In region I there is only one minimum at $\alpha = 0$. In region II there are two minima one at $\alpha = 0$ and one at $\alpha > 0$ with $V(\alpha = 0) < V(\alpha > 0)$. In region III there are two minima one at $\alpha = 0$ and one at $\alpha > 0$ with $V(\alpha = 0) > V(\alpha > 0)$. In region IV there is one maximum at $\alpha = 0$ and one minimum at $\alpha > 0$. In region V there is a minimum at $\alpha = 0$, a maximum at $\alpha > 0$ and the other minimum is at $\alpha \to \infty$. In region VI there is a maximum at $\alpha = 0$ and a minimum at $\alpha > 0$. In region VII there is a minimum at $\alpha = 0$ and a minimum at $\alpha > 0$ with $V(\alpha = 0) > V(\alpha > 0)$. In region VIII there is only a maximum at $\alpha = 0$. In region IX there is a minimum at $\alpha = 0$, a maximum at $\alpha > 0$ and the other minimum is at $\alpha \to \infty$.

![Figure 2](image-url)

Figure 2: Shown are different trajectories in the $(r_1, r_2)$ parameter space for $^{16}$O + $\alpha \to ^{20}$Ne. In the top row are the parameter spaces with the respective path of the trajectory depicted as an arrow. In the bottom row we plot the first $0^+$ energy levels as a function of the absolute value of parameter $\bar{a}$, and as an arrow also indicate the direction of the path taken. The vertical dashed line indicates the value of $\bar{a}$ where the trajectory is at the point of a phase transition: In a) crossing from region I to region IV, in b) crossing the point $(r_1 = 0, r_2 = 0)$, and in c) crossing from region II to region III. The values of the parameters used are: In a) $\bar{b} = -0.08$; in b) $r_1 = 0$; and in c) $\bar{b} = -0.036$. For all cases we used: $\xi = 0.208$ and $a = b = t_1 = 0$.

A second order QPT occurs in a trajectory in parameter space going from region I to region IV. This is because the global minimum of the potential at $\alpha = 0$ disappears and becomes a
global minimum at $\alpha > 0$ as the parameter $r_1$ goes from $r_1 > 0$ to $r_1 < 0$ at a fixed $r_2 > 0$. Following Ehrenfests’s classification of phase transitions and encountering a discontinuity in the second derivative of the global minimum with respect to the parameter $r_1$, we can conclude that the phase transition is of second order. Similarly, a third order QPT occurs in a trajectory going from $r_2 > 0$ to $r_2 < 0$ at $r_1 = 0$, passing through $r_2 = 0$, where the potential at $\alpha = 0$ goes as $\alpha^6$. Here we encounter a discontinuity in the third derivative of the global minimum of the potential with respect to the parameter $r_2$. Lastly, a first order QPT occurs in a trajectory going from region II to region III, crossing the Maxwell set. Here, the minimum at $\alpha > 0$ in region II becomes the global minimum in region III, and we encounter a discontinuity in the first derivative of the global minimum of the potential with respect to the parameters as the transition takes place.

In Fig. 2 we show examples of three different trajectories in the $(r_1, r_2)$ parameter space, with their respective plot of the first $0^+$ energy levels as a function of the absolute value of $\tilde{a}$. The trajectories in a) and c) are obtained by fixing the parameters $\xi = 0.208$, $a = b = t_1 = 0$, and using $\tilde{b} = -0.08$ and $\tilde{b} = -0.036$, respectively; the parameter $\tilde{a}$ is then varied as shown in the plots. The trajectory in b) is obtained by fixing $r_1 = 0$ and going from $r_2 > 0$ to $r_2 < 0$. For cases a) and b) avoided level crossings in the vicinity of the QPT are found, while in case c) there are no avoided level crossings. This result shows that the signatures for a phase transition depend on the path taken.

2.2.2. Deformed clusters example: $^{12}\text{C} + ^{12}\text{C} \rightarrow ^{24}\text{Mg}$

This example allows to include a deformation dependence on the clusters. We have $n_0 = 12$, $\beta_{12\text{C}} = -0.38$, $(\lambda_1, \mu_1) = (\lambda_2, \mu_2) = (0, 4)$, and $(\lambda_3, \mu_3) = (0, 8)$. In the numerical diagonalisation, up to four excitation quanta $N = 4$ are considered.

Similarly to the previous example, a second order QPT occurs as the strength of the second order Casimir operator parameter $\tilde{a}$ increases. The left plot in Fig. 3 shows the parameter space for the $^{12}\text{C} + ^{12}\text{C} \rightarrow ^{24}\text{Mg}$ system and the particular trajectory taken. The trajectory is obtained by fixing the parameters $b = -0.4$, $\xi = 0.196$, $\tilde{a} = \tilde{b} = 0$, $t_1 = 0.7175$, and varying the parameter $a$ from $a = -1.4$ to $a = -3.3$, crossing the $r_2$-axis at approximately $a = -2.0$. In the right plot we depict the $0^+_2$ and $0^+_3$ energy levels and see that the first avoided energy level crossing of the $0^+_3$ with the ground state $0^+_1$ occurs at the vicinity of the QPT. The upper turns, seen in the curve of $0^+_3$, are due to avoided level crossings with higher lying $0^+$ states, not plotted.

2.3. QPTs in a Hamiltonian with SU(3) and SO(4) symmetry: $c \neq 0$

In this case, we focus on the previous example of the system of spherical cluster $^{16}\text{O} + \alpha \rightarrow ^{20}\text{Ne}$ and this time turn on the parameter $c$, and search in the three-dimensional parameter space $(r_1, r_2, r_4)$ for a suitable trajectory. Similarly to the SU(3) limit, we fix the following parameters: $\tilde{a} = -1.06$, $\tilde{b} = -0.08$, $\xi = 0.208$, and $a = b = t_1 = 0$ and obtain the QPT trajectory varying the parameter $c$, which now crosses the $(r_2, r_4)$-plane. In Fig. 4 we show two slices of parameter space $(r_1, r_2, r_4)$ for different values of $r_4$, one at $r_4 = 0$ and the other at $r_4 = -25$, which correspond to points before and after the second order QPT, respectively.
Figure 3: In the left figure the trajectory is shown within the parameter space \((r_1, r_2)\) of a second order QPT for \(^{12}\text{C} + ^{12}\text{C} \rightarrow ^{24}\text{Mg}\) in the SU(3) limit. In the right we plot the \(0^+_2\) and \(0^+_3\) energy levels as a function of the absolute value of the parameter \(a\). Only the first three \(0^+\) states are plotted, including the ground state. Note that the \(0^+_3\) state exhibits turns which are the consequences of further crossings with higher excited states. The vertical dashed line indicates the value of \(a\) where the trajectory crosses from region I to region IV and a phase transition takes place. The values of the parameters used are: \(b = -0.4, \xi = 0.196, \bar{a} = \bar{b} = 0,\) and \(t_1 = 0.7175\). The arrow indicates the path of the trajectory.

In the left plot of Fig. 3 we can see that the change in the \(0^+_2\) and \(0^+_3\) states is now smooth and no avoided level crossings are found as the parameter \(c\) increases. However, traits of the second order QPT can still be seen elsewhere. In the middle plot of Fig. 3 we show the transition probabilities of the state \(2^+_1\) to the ground state \(0^+_1\) as a function of the parameter \(c\), where we can see a noticeable change near a critical value of \(c\). In the right plot of Fig. 3 we show the expectation value of the number of \(n_\pi\) bosons in the ground state \(\langle n_\pi(0^+_1)\rangle\) as a function of the parameter \(c\), obtained with the numerical calculation (blue) and with the coherent states (yellow). A sharp change at about \(c = 0.2\), the point of the phase transition, is present in the coherent state plot, whereas the change in the numerical calculation is smoother. The classical treatment, thus, exhibits more clearly the event of a phase transition than the exact Quantum Mechanical treatment, which includes continuous changes in the mixing of states between the two minima of the potential. This example also shows that the signature of a phase transition not always shows up clearly in the spectrum and transition values.

The behaviour seen is typical for finite quantum systems: In a strict sense, finite systems cannot exhibit a phase transition, however, a structural change can happen, with an order parameter changing significantly in a short range within the parameter space. In this example, the continuous change is explained by the formation of the two minima, i.e., the wave-function of the ground state changes its dominant contribution from the spherical minimum \((\alpha = 0)\) to the deformed minimum \((\alpha \neq 0)\) in a continuous way and no discrete jump is produced. This is different in the semi-classical description. There, a discrete jump is generated, the moment the global minimum at \(\alpha = 0\) changes to the deformed minimum at \(\alpha \neq 0\). Therefore, the phase transitions
3. Phase transitions in an effective model for QCD at low energy

The catastrophe theory not only can be applied to a nuclear cluster model but also to a topic as different as QCD. Though, QCD seems to be quite different to algebraic cluster models, it is also a many-body problem and the knowledge, acquired before, can be directly extended to this new field.

The main problem in QCD is to describe the structure of the vacuum, the lowest state in energy, which is not trivial at all. Without an interaction, the vacuum structure is simple, i.e., there are no quarks nor gluons present. However, when the interaction is switched on, the physical vacuum should contain a structure involving quarks, antiquarks and gluons (see [30]).

Instead of using the real QCD, effective models for QCD are easier to apply than a full scale non-perturbative treatment, though these effective models are non-perturbative too. One such model was proposed in [3], using a simple Hamiltonian with a structure similar to QCD. In [4, 5] a more sophisticated model was proposed, which we will use here in a modified form. The basic ingredients of this model are pairs of quark-antiquarks and of gluon pairs. As seen in Fig. 6 the interaction between those pairs are very similar as in QCD between the quarks and gluons.

The model is able to describe the low lying meson spectrum [4]. In [5] the evolution of the Quark Gluon Plasma was described. It is interesting to note that even particle-anti-particle

Figure 4: Shown are two slices of parameter space \((r_1, r_2, r_4)\) for different values of parameter \(r_4\) for the example \(^{16}\text{O} + \alpha \to ^{20}\text{Ne}\). The plot in the left corresponds to a point before the QPT at \(c = 0\). The plot in the right corresponds to a point after the QPT at \(c = 0.6\). In both cases an inset with the corresponding semi-classical potential is shown. The values of the parameters used are: \(\bar{a} = -1.06\), \(\bar{b} = -0.08\), \(\xi = 0.208\), and \(a = b = t_1 = 0\).
production rates could be reproduced. In [6] hadron states were also described well, while also Penta-Quark and Hepta-Quark states were predicted.

We follow the model described in [4], with a different trial state, implying a modification in the structure of the interaction. The energy scales of the model are depicted in Fig. 7, which defines the scale of the fermion and boson states. The scale of the fermionic state is $\omega_q = 0.33$ GeV, a value chosen because three times this value should give approximately the mass of the nucleon state, i.e., of 1 GeV. Each fermionic state has a degeneracy of $2\Omega = 18$ (3 color, 3 flavour and 2 spin degrees of freedom). A Dirac picture is employed: In the perturbative vacuum the lowest fermion level, at $-\omega_q$, is fully occupied. Excited states are obtained by lifting quarks from the lower to the higher level, creating a particle-hole state. A hole is described as an antiquark, i.e., a particle-hole state corresponds to a quark-antiquark state.

The Hamiltonian of the model is

$$H = 2\omega_q n_q + \omega_\beta n_\beta + C \left\{ \left[ (b^\dagger)^2 s^2 + 2(b^\dagger \cdot b) + (s^\dagger)^2 b^2 \right] \left( 1 - \frac{n_\beta}{2\Omega} \right) \beta^\dagger \right. \right.$$ 

$$+ \left. \beta \left[ (b^\dagger)^2 s^2 + 2(b^\dagger \cdot b) + (s^\dagger)^2 b^2 \right] \right\} ,$$

(22)

where $n_q$ is the number of quark-antiquarks (particle-hole) pairs, $n_\beta$ the number gluon pairs, $b^\dagger$, $b$ are the quark-antiquark pair creation and annihilation operators and $\beta^\dagger$, $\beta$ are the same for the gluon pairs. The parameter $C$ gives the intensity of the interaction. When $C = 0$ there is no interaction and the ground state is always given by all pairs of quarks in the lower level and no gluon pairs. The factor $\left( 1 - \frac{n_\beta}{2\Omega} \right)$ considers the PEP by shutting off the interaction when all quarks are excited to the upper fermion level, thus, no further excitation can take place. In Fig. 6 we depict the graphical presentation of the interactions in (22) in terms of double straight lines for the quark-antiquark pairs and by double wavy lines for the gluon pairs.

The coherent state is defined as:

$$|\psi\rangle = N_q N_\beta e^{\gamma^\dagger} \left[ \begin{array}{c} s^\dagger + (\alpha \cdot b)^\dagger \end{array} \right]^{2\Omega} |0\rangle ,$$

(23)
where $N_q$ and $N_\beta$ are normalization factor for the fermions and bosons, respectively, given by

$$N_q = \frac{1}{\left[\frac{(2\Omega)!}{(1 + (\alpha^* \cdot \alpha))^{2\Omega}}\right]^{\frac{1}{2}}}$$

$$N_\beta = e^{-\frac{\gamma^* \gamma}{2}}.$$ (24)

The vacuum state $|0\rangle = |0\rangle_q |0\rangle_\beta$ is the direct product of the fermion and boson vacuum. In [3] a different coherent state was used. The one in (23) is inspired by a collective model in nuclei: The basic elements are pairs of fermions which behave as bosons. The Pauli exclusion principle is taken into account by the maximal number of particle-hole pairs which can be created, as explained above. One introduces an auxiliary scalar boson ($s$) and requires that the sum of $s$ and $b$ bosons is constant, given by $2\Omega$. In the perturbative vacuum the state below 0 is fully occupied, which in the effective model corresponds to having 18 quarks in the lowest state (Dirac picture). Because the total number of particles in the Dirac picture is $2\Omega = n_s + n_b$ ($n_s$ is the number of $s$-bosons and $n_b$ is the number of $b$-bosons), the number of quark-antiquark pairs vary from 0 to $2\Omega$. The model does not include orbital degrees of freedom. If more quark-antiquarks pairs are needed, one has to include these orbital degrees of freedom.

In a similar fashion we obtain the semi-classical potential $V = \langle H \rangle$ as the expectation value
of the Hamiltonian (22) in the basis of coherent states (23): 

\begin{equation}
V = 2\omega_q(2\Omega) \left[ \frac{(\alpha^* \cdot \alpha)}{[1 + (\alpha^* \cdot \alpha)]^2} + \omega_\beta \gamma^* \gamma + 2\Omega(2\Omega - 1)C(\gamma + \gamma^*) \left[ \frac{(\alpha \cdot \alpha) + (\alpha^* \cdot \alpha^*)}{[1 + (\alpha^* \cdot \alpha)]^2} \right] \right] + \frac{2}{2\Omega - 1} \left[ \frac{(\alpha^* \cdot \alpha)}{[1 + (\alpha^* \cdot \alpha)]^2} \right] \left( 1 - \frac{(\alpha^* \cdot \alpha)}{1 + (\alpha^* \cdot \alpha)} \right). \tag{25}
\end{equation}

Using the following parametrization of the coherent states:

\begin{align*}
(\alpha \cdot \alpha) &= \alpha_{(0,0)}^2 e^{2i\phi_{(0,0)}} + \alpha_{(1,1)}^2 e^{2i\phi_{(1,1)}} \\
(\alpha^* \cdot \alpha) &= \alpha_{(0,0)}^2 + \alpha_{(1,1)}^2 \\
(\alpha^* \cdot \alpha^*) &= (\alpha_{(0,0)}^2 e^{-2i\phi_{(0,0)}} + \alpha_{(1,1)}^2 e^{-2i\phi_{(1,1)}} \\
\gamma &= \gamma e^{i\phi_\gamma}
\end{align*}

we can rewrite the semi-classical potential as

\begin{align*}
V &= 2\omega_q(2\Omega) \left[ \frac{\alpha_{(0,0)}^2 + \alpha_{(1,1)}^2}{1 + \alpha_{(0,0)}^2 + \alpha_{(1,1)}^2} \right] + \omega_\beta \gamma^2 \\
&+ 2\Omega(2\Omega - 1)C\gamma(e^{i\phi_\gamma} + e^{-i\phi_\gamma}) \left[ \frac{\alpha_{(0,0)}^2 (e^{2i\phi_{(0,0)}} + e^{-2i\phi_{(0,0)}}) + \alpha_{(1,1)}^2 (e^{2i\phi_{(1,1)}} + e^{-2i\phi_{(1,1)}})}{1 + \alpha_{(0,0)}^2 + \alpha_{(1,1)}^2} \right] \\
&+ \omega_\beta \gamma^2.
\end{align*}

Figure 7: This figure depicts the relative position of the quark and gluon states. The quark sector is described by a Lipkin model, consisting of two levels at ±ω_q. The value of ω_q is 0.33 GeV, i.e., three times of that value reproduces approximately the mass of a nucleon. The gluon state is at 1.6 GeV, corresponding to the energy of two gluons, with the one-gluon energy of 0.8 GeV.
\[ V = 2\omega_q(2\Omega) - \frac{\alpha^2}{(1+\alpha^2)^2} + \omega_\beta \gamma^2 \\
+2\Omega(2\Omega-1)C2\gamma \cos \phi_\gamma \left[ \frac{2\alpha_{(0,0)}^2 \cos 2\phi_{(1,1)} + 2\alpha_{(1,1)}^2 \cos 2\phi_{(1,1)}}{1+\alpha^2} \right] \\
+\frac{2}{2\Omega - 1 + \alpha^2} \left( 1 - \frac{\alpha^2}{1+\alpha^2} \right), \tag{27} \]

where we defined \( \alpha_{(0,0)}^2 + \alpha_{(1,1)}^2 \equiv \alpha^2 \) as a new variable. The \( \alpha_{(\lambda,\mu)} \) refer to the coupling of a quark-antiquark to a definite flavour irrep, where \((0,0)\) is flavour zero and \((1,1)\) is the flavour octet. The structure of the potential is similar to the one of the SACM, save with simpler \( F_{pq}(\alpha) \)-functions. For a given \( \alpha^2 \), the \( \alpha_{(0,0)}^2 \) can vary from 0 to \( \alpha^2 \) and so in the opposite manner also the \( \alpha_{(1,1)}^2 \), which is a symmetry property of the model.

We now continue with the minimization of the potential. The critical points of the angular variables are easily obtained, i.e., they are given by \( \phi_\gamma = \phi_{(0,0)} = \phi_{(1,1)} = 0 \). The semi-classical potential is then a function of two variables:

\[ V(\alpha, \gamma; C) = 4\Omega\omega_q \frac{\alpha^2}{(1+\alpha^2)^2} + \omega_\beta \gamma^2 + 8\Omega(2\Omega-1)C\gamma \frac{\alpha^2}{(1+\alpha^2)^2} \left[ \frac{1}{1+\alpha^2} + \frac{2}{2\Omega - 1} \right]. \tag{28} \]

The potential has a quadratic dependence on the variable \( \gamma \). The critical points of the potential satisfy \( \nabla V(\alpha_c, \gamma_c) = 0 \). The component for the variable \( \gamma \) is the partial derivative

\[ \left. \frac{\partial V}{\partial \gamma} \right|_{\gamma_c} = 2\omega_\beta \gamma_c + 8\Omega(2\Omega-1)C\gamma \frac{\alpha^2}{(1+\alpha^2)^2} \left[ \frac{1}{1+\alpha^2} + \frac{2}{2\Omega - 1} \right] = 0, \tag{29} \]

and solving for \( \gamma_c \) we obtain

\[ \gamma_c = -4\Omega(2\Omega-1)C \frac{\alpha^2}{\omega_\beta (1+\alpha^2)^2} \left[ \frac{1}{1+\alpha^2} + \frac{2}{2\Omega - 1} \right]. \tag{30} \]

Direct substitution of (30) in (28) permits us to write the one dimensional potential as

\[ V(\alpha, \gamma_c; C) = 4\Omega\omega_q \left\{ \frac{\alpha^2}{(1+\alpha^2)^2} - \kappa \frac{\alpha^4}{(1+\alpha^2)^4} \left[ \frac{1}{1+\alpha^2} + \frac{2}{2\Omega - 1} \right]^2 \right\}. \tag{31} \]

The dimensionless parameter \( \kappa \) is defined as

\[ \kappa = 4\Omega(2\Omega-1)^2 \frac{C^2}{\omega_\beta \omega_\beta}. \tag{32} \]
Figure 8: Global minimum of the semi-classical potential as a function of $\kappa$. At $\kappa = 8.14502$ ($C = 0.020331$ GeV) a first order phase transition occurs. A discontinuity in the first derivative with respect to $\kappa$ can be seen in the plot. We used the values $\omega_q = 0.33$ GeV, $\omega_\beta = 1.6$ GeV and $2\Omega = 18$.

3.1. Bifurcation and Maxwell sets

In the one dimensional parameter space $\kappa$ the bifurcation and Maxwell sets can be obtained by direct application of the formulas in Appendix A.

The critical manifold is the surface of critical points spanned by the variation of parameter $\kappa$. The critical points are those that satisfy

$$\frac{\partial V(\alpha, \gamma; C)}{\partial \alpha} = 0.$$  \hfill (33)

This potential exhibits an interesting feature. The Hessian determinant of the potential (28) at $\alpha = 0$ and $\gamma = 0$ is given by

$$\begin{vmatrix}
\frac{\partial^2 V(\alpha, \gamma; C)}{\partial \alpha^2} & \frac{\partial^2 V(\alpha, \gamma; C)}{\partial \alpha \partial \gamma} \\
\frac{\partial^2 V(\alpha, \gamma; C)}{\partial \gamma \partial \alpha} & \frac{\partial^2 V(\alpha, \gamma; C)}{\partial \gamma^2}
\end{vmatrix}_{(\alpha=0, \gamma=0)} = 16\Omega \omega_q \omega_\beta,$$  \hfill (34)

and we can see that it is always positive. In other words, the semi-classical treatment gives a potential which maintains a local minimum at the origin ($\alpha = 0, \gamma = 0$), even after the phase transitions, which corresponds to the perturbative vacuum. A local minimum is related to an excited state, i.e. the perturbative vacuum still persists as an excited state at higher energies.

We solve (33) for $\kappa$ and get

$$\kappa = -\frac{(1 - \alpha^2)(1 + \alpha^2)^4(2\Omega - 1)^2}{2\alpha^2(\alpha^2 + 2\Omega)(\alpha^4 + 2\alpha^2(2\Omega - 1) - 2\Omega)},$$  \hfill (35)
The singular mapping to the parameter space happens when the derivative of (35) with respect to $\alpha$ is zero. This condition leads to a 10th degree polynomial:

$$f_B(\alpha, 2\Omega) = -4\Omega^2 + 4\Omega\alpha^2(7\Omega - 3) - 2\alpha^4(20\Omega^2 - 18\Omega + 3) + 2\alpha^6(12\Omega^2 - 18\Omega + 5) + \alpha^8(12\Omega - 7) + \alpha^{10},$$

(36)

whose solution is to be substituted in (35) to get the bifurcation set. For the set values of $\omega_q = 0.33$ GeV, $\omega_\beta = 1.6$ GeV and $2\Omega = 18$, we obtain

$$\kappa_B = 5.8997,$$

(37)

and using the definition (32) we return to the original parameter $C$:

$$C_B = 0.017303$$

(38)

To obtain the Maxwell set we consider the roots of the potential

$$V(\alpha, \gamma_c; C) + V_0 = 0,$$

(39)

and define the roots manifold as the surface spanned by the variation of parameter $\kappa$ of all the real roots satisfying (39). The Maxwell set will be the one obtained where the mapping of this surface to the parameter space is singular.

We solve for $\kappa$ in (39), setting $V_0 = 0$ (as no two minima coincide at $V_0 \neq 0$ for the potential (31)), and get

$$\kappa = \frac{(1 + \alpha^2)^4(2\Omega - 1)^2}{\alpha^2(\alpha^2 + 2\Omega)^2}.$$

(40)

The singular mapping to the parameter space happens when the derivative of (40) with respect to $\alpha$ is zero. This condition leads to a 4th degree polynomial:

$$f_M(\alpha, 2\Omega) = -2\Omega + 3\alpha^2(2\Omega - 1) + \alpha^4.$$

(41)

The appropriate real solutions are given by

$$\alpha = \pm \sqrt{\frac{1}{2} \left( -3(2\Omega - 1) + \sqrt{36\Omega^2 - 28\Omega + 9} \right)}$$

(42)

and substituting in (40) we obtain the Maxwell set as a function of $2\Omega$. For completeness we write the explicit expression:

$$\kappa_M(2\Omega) = \frac{(2\Omega - 1)^2 \left( 5 - 6\Omega + \sqrt{9 + 4\Omega(9\Omega - 7)} \right)^4}{2 \left( 3 - 6\Omega + \sqrt{9 + 4\Omega(9\Omega - 7)} \right) \left( 3 - 2\Omega + \sqrt{9 + 4\Omega(9\Omega - 7)} \right)^2}.$$

(43)

For the set values of $\omega_q = 0.33$ GeV, $\omega_\beta = 1.6$ GeV and $2\Omega = 18$, we get

$$\kappa_M = 8.14502,$$

(44)
and using the definition (32) we return to the original parameter $C$:

$$C_M = 0.020331 \text{GeV.}$$

(45)

In Fig. 8 we plot the global minimum of the potential as a function of $\kappa$. The point of the phase transition is given by the kink a little above $\kappa = 8$. At this point, a former excited $0^{++}$ (The notation is $J^{PC}$, with the spin $J$, parity $P$ and charge conjugation $C$) state, with the same quantum numbers as the perturbative vacuum, crosses the perturbative vacuum, being the new vacuum state, which contains a finite number of quark-antiquark pairs and pairs of gluons.

In Fig. 9 we show the contour plots of the two-dimensional semi-classical potential (28) for different values of $C$, along with the critical value for $\gamma$ given in (30) and indicated by a solid blue line. The corresponding one-dimensional semi-classical potentials (31) are also plotted. As the intensity of the parameter increases, passing the critical value $C_M$ (45), the global minimum is no longer at $\alpha = 0$ and a first order quantum phase transition occurs. The jump occurs at the same point as in Fig. 8.

![Figure 9: Contour plots ($\alpha, \gamma$) of the semi-classical potential (28) for different values of parameter $C$ with their corresponding one dimensional semi-classical potential (31). The blue line in the left panel corresponds to the critical values of $\gamma_c$ as a function of $\alpha$ given in (31). We used the values $\omega_\eta = 0.33 \text{GeV}$, $\omega_\beta = 1.6 \text{GeV}$ and $2\Omega = 18$.](image)

For small $C$ the global minimum is at $\alpha = 0$, where we do not take into account the asymptotic minimum for $\alpha \to \infty$. Then, with increasing $C$ a second minimum forms, first at
larger energies than the one at $\alpha = 0$. The Maxwell point is reached when both minima are at the same height. For even larger $C$ the global minimum is a deformed one ($\alpha > 0$), but still maintaining an excited minimum at $\alpha = 0$. A local minimum indicates the existence of the state, i.e., the model predicts that after the phase transition the former perturbative vacuum state still exists as an excited state. This is in accordance to [4], where the $f_0(400-1200)$ state has a content of half a quark-antiquark and half a gluon pair (the non-integer number refers to the expectation number of the pair operators with respect to the state function). That such a property emerges in this particular model is a novelty, indicating that the use of coherent states can give more information than just the ground state properties.

3.1.1. Some consequences

The expectation number of the quarks and gluons pairs are, respectively:

$$\langle n_q \rangle = 2\Omega \frac{\alpha^2}{1 + \alpha^2},$$
$$\langle n_\beta \rangle = \gamma^2.$$  \hspace{1cm} (46)

In Fig. 10 these values are plotted as a function of parameter $C$. The plots are obtained by evaluating $\langle n_q \rangle$ and $\langle n_\beta \rangle$ at the critical point $(\alpha_c, \gamma_c)$ of the global minimum of the semi-classical potential. A discontinuity is present at the point of the first order phase transition $C = 0.020331$ GeV. At about $C = 0.039$ GeV the gluon number surpasses the quarks. With increasing interaction ($C$), the number of quark-antiquark pairs becomes saturated, while the gluon pairs continue to rise, winning over the quark-antiquark pairs.

In [31] a relation of the quark-antiquark and gluon condensate [30] to the number of quark-antiquark and gluon pairs in the physical vacuum $|\text{vac}\rangle$ was given, namely

$$\langle \text{vac}|\bar{\Psi}_f \Psi_f |\text{vac}\rangle = \frac{1}{V} \left( \frac{2n_q}{3} - 6 \right),$$
$$\langle \text{vac}|\bar{\Omega}_s F^a_{\mu \nu} F^a_{\mu \nu} |\text{vac}\rangle = \left( \frac{\alpha_s 16\pi}{\omega_\beta V^2} \right) (4n_\beta + 9).$$  \hspace{1cm} (47)

The $\Psi_f$ is the fermion function and $V = \frac{4\pi}{3}r_0^3$ is the volume of the size of a hadron with radius $r_0 = 0.875$ fm = 4.375 GeV$^{-1}$ [31]. The $\alpha_s$ is the strong coupling constant. The values of the quark and gluon condensates in [30] are

$$\langle \text{vac}|\bar{\Psi}_f \Psi_f |\text{vac}\rangle \approx -(0.223 \text{ GeV})^3,$$
$$\langle \text{vac}|\bar{\Omega}_s F^a_{\mu \nu} F^a_{\mu \nu} |\text{vac}\rangle \approx (0.360 \text{ GeV})^4.$$  \hspace{1cm} (48)

The first condition with (47) leads to $n_q \approx 4$. Comparing this number to Fig. 10 we can identify this number to be approximately realized just after the phase transition took place. Thus we selected two points near this value: In Fig. 10 two positions just after the phase transition are indicated by a dot (with $C_M = C_1 = 0.020331$ GeV) and by a star (with $C_2 = 0.022301$ GeV). For the point $C_M$ the expectation values are $\langle n_q \rangle = 4.67192$, $\langle n_\beta \rangle = 1.42697$. They lead to
for the quark condensate. For the gluon condensate we solve for \( \alpha_s \), obtaining \( \alpha_s = 7.156 \), not very far from the value deduced in [31] and also in good agreement with [30]. For the star value \( C_2 \) the same procedure, with \( \langle n_q \rangle = 5.01946 \) and \( \langle n_\beta \rangle = 1.79012 \), leads to the quark condensate value \(- (0.1963 \text{ GeV})^3\), a little lower than in the former case, and to the strong coupling constant \( \alpha_s = 6.513 \), a little lower than in the former case.

![Figure 10: Expectation values of quarks pairs \( \langle n_q \rangle \) (blue, solid) and gluon pairs \( \langle n_\beta \rangle \) (yellow, dashed) as a function of the parameter \( C \). The dots represent the number of quarks pairs and gluon pairs at the Maxwell set \( C = 0.020331 \text{ GeV} \). The stars represent the number of quarks pairs and gluon pairs at \( C = 0.022301 \text{ GeV} \). We used the values \( \omega_q = 0.33 \text{ GeV}, \omega_\beta = 1.6 \text{ GeV} \) and \( 2\Omega = 18 \).](image)

This last calculation shows that the model is consistent, that the catastrophe theory is a helpful guide to describe the phase transition and that the physical vacuum is probably a state near the point of a phase transition.

4. Conclusions

One motivation of this contribution was to extend a cluster model (the SACM) to include deformation dependencies in the clusters and to correlate signatures in the spectrum with phase transitions. Another motivation was to show that the catastrophe theory has a wide range of practical applications to different areas in physics, such as QCD, which was the second example discussed in this contribution. Applications to Optics and General Relativity were mentioned earlier in the Introduction.

In the case of the SACM we showed the effectiveness of the catastrophe theory to describe a very complicated semi-classical potential, where deformation effects were included. Phase transitions up to 3rd order were encountered, depending also on the path taken in the phase transitions.
space. It was possible to identify quantum phase transitions effects when a numerical calculation of the spectrum was performed. Changes in the spectrum as a function of an interaction parameter corresponded to a transition from one region in parameter space to another, where the global minimum of the semi-classical potential changes from spherical to deformed. It was found that the changes in the numerical calculations of the transition probability and the expectation value of the number of \( n_\pi \) bosons were smooth, while in the semi-classical description the changes were clearly marked by a jump in the structure. This is due to the fact that in a Quantum Mechanical treatment the wave function changes smoothly from one minimum to the other, while in the semi-classical treatment the jump happens when one minimum is below the other.

As a second example the phase transition of an effective model of QCD was investigated, describing how the perturbative vacuum changes to a vacuum with a content of quark-antiquark pairs and gluons pairs. The phase transition is of first order.

We hope that the motivation of the importance and effectiveness of the catastrophe theory formalism to the study of phase transitions, along with the techniques described here, will encourage the reader to apply it in other areas of interest.

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Appendix A. General expressions for the bifurcation set and Maxwell set

In some steps the software MATHEMATICA [29] was used to simplify some expressions.

Let us consider a one dimensional real function \( V(x; r_1, r_2, r_3) \) dependent on three real parameters \( r_i \) of the form

\[
V(x; r_1, r_2, r_3) = r_1 g_1(x) + r_2 g_2(x) + r_3 g_3(x) + g_4(x),
\]

where \( g_j(x) \), \( j = 1, 2, 3, 4 \), are arbitrary rational functions with no singularities in the domain of \( x \).

The bifurcation set is the subspace in parameter space \((r_1, r_2, r_3)\), where the mapping \((x_c, r_1, r_2, r_3) \mapsto (r_1, r_2, r_3)\) of the critical manifold to the parameter space is singular, i.e., when the Jacobian determinant of this transformation vanishes [2]. The bifurcation set serves as the separatrix where critical points begin to emerge.

The critical manifold is the surface of all critical points spanned by the variation of parameters satisfying

\[
\left. \frac{dV}{dx} \right|_{x=x_c} = r_1 g_1'(x_c) + r_2 g_2'(x_c) + r_3 g_3'(x_c) + g_4'(x_c) = 0.
\]

From (A.2) we can solve for \( r_1 \) and obtain

\[
r_1 = -\frac{1}{g_1'(x_c)} \left( r_2 g_2'(x_c) + r_3 g_3'(x_c) + g_4'(x_c) \right),
\]

(3)
which allows us to express the parameter \( r_1 \) as a function of the critical points \( x_c \) and the parameters \( r_2 \) and \( r_3 \); thus, the mapping of the critical manifold to the parameter space becomes \((x_c, r_2, r_3) \mapsto (r_1, r_2, r_3)\). Then, the Jacobian determinant of the mapping of the critical manifold to the parameter space is given by

\[
\begin{vmatrix}
\frac{\partial x_1}{\partial x_c} & \frac{\partial x_1}{\partial r_2} & \frac{\partial x_1}{\partial r_3} \\
\frac{\partial x_2}{\partial x_c} & \frac{\partial x_2}{\partial r_2} & \frac{\partial x_2}{\partial r_3} \\
\frac{\partial x_3}{\partial x_c} & \frac{\partial x_3}{\partial r_2} & \frac{\partial x_3}{\partial r_3}
\end{vmatrix} = \begin{vmatrix}
\frac{\partial r_1}{\partial x_c} & \frac{\partial r_1}{\partial r_2} & \frac{\partial r_1}{\partial r_3} \\
0 & 1 & 0 \\
0 & 0 & 1
\end{vmatrix} = \frac{\partial r_1}{\partial x_c}. \tag{A.4}
\]

The mapping is singular when the Jacobian determinant vanishes. Using \((A.3)\) we have

\[
\frac{\partial r_1}{\partial x_c} = \frac{1}{(g_1'(x_c))^2} \left( r_2 W(g_2', g_1') + r_3 W(g_3', g_1') + W(g_4', g_1') \right) = 0, \tag{A.5}
\]

where \( W(f, g) = f(x)g'(x) - f'(x)g(x) \) is the Wronskian determinant. We solve for \( r_2 \) in \((A.5)\) and obtain

\[
r_2 = -\frac{1}{W(g_1', g_2') \left( r_3 W(g_1', g_3') + W(g_1', g_4') \right)}, \tag{A.6}
\]

as a function of parameter \( r_3 \) and of the critical points \( x_c \). Direct substitution of \((A.6)\) in \((A.3)\) gives us \( r_1 \) as a function of parameter \( r_3 \) and of the critical points \( x_c \) as

\[
r_1 = \frac{1}{W(g_1', g_2')} \left( r_3 W(g_1', g_3') + W(g_2', g_4') \right). \tag{A.7}
\]

The parametric surface in three-dimensional space defined by \((A.6)\) and \((A.7)\):

\[
\mathcal{C}_B = \{(r_1(x_c; r_3), r_2(x_c; r_3), r_3) \mid x_c, r_3 \in \mathbb{R}\} \tag{A.8}
\]

is the bifurcation set of the potential function \((A.1)\).

The Maxwell set is the subspace in parameter space where for at least two critical points \( x_1 \) and \( x_2 \) the following condition holds

\[
V(x_1; r_1, r_2, r_3) = V(x_2; r_1, r_2, r_3) = -V_c, \tag{A.9}
\]

i.e. the value of the function at two critical points \( x_1 \) and \( x_2 \) is the same and equal to \(-V_c\), with \( V_c \in \mathbb{R} \).

This persuade us to consider the roots manifold, defined as the manifold of all the real roots \( x_r \) spanned by the variation of parameters satisfying

\[
V(x_r; r_1, r_2, r_3) + V_c = 0. \tag{A.10}
\]

When the parameters are varied arbitrarily a critical point occurs when two real roots (or a conjugate complex pair) of \((A.10)\) coalesce. Thus, we consider the case when the mapping of the roots manifold \((A.10)\) to the parameter space is singular, which corresponds precisely to the coalescence of two roots. We solve for \( r_1 \) in \((A.10)\) and obtain:

\[
r_1 = -\frac{1}{g_1(x_r)} \left( r_2 g_2(x_r) + r_3 g_3(x_r) + g_4(x_r) + V_c \right). \tag{A.11}
\]
Analogous to (A.4), the Jacobian determinant of the transformation is

\[
\frac{\partial r_1}{\partial x_r} = \frac{1}{g^2_1(x_r)} \left( r_2 W(g_2, g_1) + r_3 W(g_3, g_1) + W(g_4, g_1) + g'_1(x_r)V_c \right),
\]

(A.12)

and the singular mapping occurs when it vanishes. This allows us to solve for \(r_2\) and obtain

\[
r_2 = -\frac{1}{W(g_1, g_2)} \left( r_3 W(g_1, g_3) + W(g_1, g_4) - g'_1(x_r)V_c \right),
\]

(A.13)

which is given in terms of the critical points \(x_r\) and the parameter \(r_3\) and \(V_c\). Direct substitution of (A.13) in (A.11) allows us to obtain \(r_1\) in terms of the same values as \(r_2\):

\[
r_1 = \frac{1}{W(g_1, g_2)} \left( r_3 W(g_2, g_3) + W(g_2, g_4) - g'_2(x_r)V_c \right).
\]

(A.14)

Equations (A.13) and (A.14) provide the values of \(r_1\) and \(r_2\) for which there exists a critical point \(x_r\) such that \(V(x_r; r_1, r_2, r_3) = -V_c\) for \(r_3\) fixed. We can show that the \(x_r\), which satisfy both (A.13) and (A.14), are critical points by direct substitution in (A.2) with \(x_c = x_r\).

Condition (A.9) for the Maxwell set is equivalent to demand that there exist two different values \(x_1\) and \(x_2\) for which the following set of algebraic equations are simultaneously satisfied:

\[
\begin{align*}
    r_2(x_1; r_3, V_c) &= r_2(x_2; r_3, V_c) \\
    r_1(x_1; r_3, V_c) &= r_1(x_2; r_3, V_c),
\end{align*}
\]

(A.15)\hspace{1cm} (A.16)

with \(r_2\) and \(r_1\) given by (A.13) and (A.14), respectively. We can rewrite (A.15) and (A.16) as the following set of equations:

\[
\begin{align*}
    r_2 : & \quad r_3 W_{13}(x_1, x_2) + W_{14}(x_1, x_2) - V_c G_1(x_1, x_2) = 0 \quad (A.17) \\
    r_1 : & \quad r_3 W_{23}(x_1, x_2) + W_{24}(x_1, x_2) - V_c G_2(x_1, x_2) = 0 \quad (A.18)
\end{align*}
\]

where we defined the following functions:

\[
\begin{align*}
    W_{ij}(x_1, x_2) &= W(g_i, g_j)|_{x_1} W(g_1, g_2)|_{x_2} - W(g_i, g_j)|_{x_2} W(g_1, g_2)|_{x_1} \quad (A.19) \\
    G_i(x_1, x_2) &= g'_i(x_1) W(g_1, g_2)|_{x_2} - g'_i(x_2) W(g_1, g_2)|_{x_1}. \quad (A.20)
\end{align*}
\]

The system of equations (A.17) and (A.18) can be solved by eliminating \(V_c\) and obtaining \(r_3\) as a function of \(x_1\) and \(x_2\), and also by eliminating \(r_3\) and obtaining \(V_c\) as a function of \(x_1\) and \(x_2\). Eliminating \(V_c\) from (A.17) and (A.18) we obtain:

\[
\begin{align*}
    r_3 \left( G_2(x_1, x_2) W_{13}(x_1, x_2) - G_1(x_1, x_2) W_{23}(x_1, x_2) \right) \\
    + G_2(x_1, x_2) W_{14}(x_1, x_2) - G_1(x_1, x_2) W_{24}(x_1, x_2) = 0,
\end{align*}
\]

(A.21)

and eliminating \(r_3\) from (A.17) and (A.18) we get:

\[
\begin{align*}
    V_c \left( G_1(x_1, x_2) W_{23}(x_1, x_2) - G_2(x_1, x_2) W_{13}(x_1, x_2) \right)
\end{align*}
\]
The combinations of functions appearing in (A.21) and (A.22) can be written as follows:

\[ G_2(x_1, x_2)W_{11}(x_1, x_2) - G_1(x_1, x_2)W_{20}(x_1, x_2) \]
\[ = W(g_1, g_2)|_{x_1} W(g_1, g_2)|_{x_2} \left( g'_1(x_1) W(g_2, g_1)|_{x_2} + g'_1(x_2) W(g_2, g_1)|_{x_1} \right) \]
\[ - g'_2(x_1) W(g_1, g_1)|_{x_2} - g'_2(x_2) W(g_1, g_1)|_{x_1} + g'_i(x_1) W(g_1, g_2)|_{x_2} + g'_i(x_2) W(g_1, g_2)|_{x_1}, \]

and

\[ W_{23}(x_1, x_2)W_{14}(x_1, x_2) - W_{13}(x_1, x_2)W_{24}(x_1, x_2) \]
\[ = - W(g_1, g_2)|_{x_1} W(g_1, g_2)|_{x_2} \left( W(g_1, g_2)|_{x_1} W(g_3, g_4)|_{x_2} + W(g_1, g_2)|_{x_2} W(g_3, g_4)|_{x_1} \right) \]
\[ - W(g_1, g_3)|_{x_1} W(g_2, g_4)|_{x_2} - W(g_1, g_3)|_{x_2} W(g_2, g_4)|_{x_1} \]
\[ + W(g_1, g_4)|_{x_1} W(g_2, g_3)|_{x_2} + W(g_1, g_4)|_{x_2} W(g_2, g_3)|_{x_1}. \]

Note that (A.23) and (A.24) simplify both (A.21) and (A.22) because the common term \( W(g_1, g_2)|_{x_1} W(g_1, g_2)|_{x_2} \) can be factored out of the equations.

Once \( x_1 \) and \( x_2 \) are determined from (A.21), for a given value of \( r_3 \), we obtain the respective value of \( V_c \) from (A.22). Finally, we substitute it all back in (A.13) and (A.14), so that now \( r_1 \) and \( r_2 \) are given in terms of \( x_1, x_2 \) and \( r_3 \), and obtain the Maxwell set as the parametric surface in three-dimensional space defined as:

\[ \mathcal{C}_M = \{(r_1(x_1, x_2; r_3), r_2(x_1, x_2; r_3), r_3) \mid x_1, x_2, r_3 \in \mathbb{R}\}, \]

with \( x_1 \) and \( x_2 \) satisfying (A.15) and (A.16). In the simple case where the function (A.1) has an extremum at \( V_c = 0 \), it suffices to use (A.13) and (A.14).

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