

# Results on quantum phase transitions within the semimicroscopic algebraic cluster model and extension to deformed clusters

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**Abstract.** The properties of quantum phase transitions in the semimicroscopic algebraic cluster model are investigated. The order of the quantum phase transition is shown to depend on the path taken in the parameter space and a novel procedure to obtain the Maxwell set separatrix is discussed. The first steps toward a description of systems of deformed cluster and heavy nuclei are presented.

## 1. Introduction

Research on quantum phase transitions (QPT) in nuclear systems has a long tradition [1]. It has been studied in the *Interacting Boson Approximation* (IBA) [2], in boson systems with an arbitrary number of bosons [3], and in the *Semimicroscopic Algebraic Cluster Model* (SACM) [4]. In these studies, the Hamiltonians used have a simple structure containing up to second order interactions, and in order to study QPTs a potential is constructed as the expectation value of the Hamiltonian in the coherent states basis of the system. This potential represents a semi-classical approximation and it is susceptible to a stability structure analysis of the physical system in terms of its parameters.

However, for models studied in the past the semi-classical potentials obtained are relatively simple. In contrast, in the SACM the semi-classical potential is quite complicated due to the coherent state, which reflects the Wildermuth condition [5], which is necessary for the observation of the Pauli exclusion principle. This kind of complicated potential was investigated in [4, 6] and may serve as an example for other potentials of similar complexity, that originate in physical systems of interest to the community.

For a complete investigation of QPTs within the SACM we use the catastrophe theory [7], which was already applied with great success to the IBA-I Hamiltonian [8]. In [6] we presented the results of this investigation and showed how the catastrophe theory can help to obtain analytical solutions for systems with an involved structure (see comments at the end of Section 2). This contribution is meant to give a brief review on these methods, summarizing the results of [6] and extending the treatment to include systems of deformed clusters.



In the Section 2 we give a brief summary of what is the essence of *catastrophe theory* [7] and what is the advantage of using this theory. Section 3 gives an account of the SACM and its main characteristics. In section 4 some of the main results will be presented. In section 5 an extension when dealing with systems of deformed clusters will be introduced in preparation for future work. Finally, in section 6 conclusions will be drawn.

## 2. Brief summary to catastrophe theory

The physical system of interest is usually described by a Hamiltonian, depending on some interaction parameters. The expectation value of this Hamiltonian with respect to a trial state defines a semi-classical potential, depending also on the interaction parameters. The variables are related to some physical object: For example, the variable  $\alpha$ , in the example presented here, is related to the distance between the two clusters [6, 9].

Important information of the physical properties of the system can be obtained by studying the stability structure of the potential and how their extrema depend on the change of the parameters. The straightforward approach consist in finding the critical points, calculating the Hessian matrix to find whether they are maxima, minima or saddle points, and so on. In practice this approach may lead to not very friendly expressions to solve analytically.

Catastrophe theory is a program to determine the dependence of parameters on the critical points of a function, thus, avoiding to get the variables at the critical points as a function of the parameters. An essential concept of catastrophe theory is that of the critical manifold, which is an hypersurface of all the critical points of the function spanned by the continuous variation of the parameters.

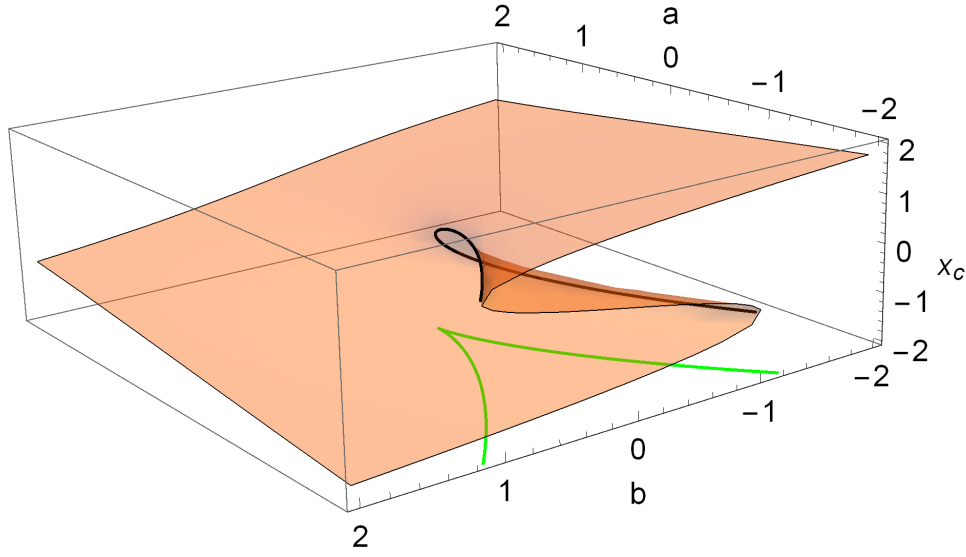
The essence of catastrophe theory lies in the singular mapping of the critical manifold to the parameter space. In Fig. 1 the critical manifold of the elementary *cusp catastrophe* [7] is shown, the singular mapping occurs when the tangent plane to the surface is vertical, i.e. when the Jacobian determinant of the transformation vanishes. The result of the application of catastrophe theory is the division of the parameter space in regions where the qualitative behavior of the potential is the same. For example, the set of points in the parameter space obtained by the projection of the points where the tangent plane to the critical manifold is vertical is known as the bifurcation set separatrix, which determines the emergence of critical points. In Section 3 the method used to calculate the Maxwell set separatrix, based on catastrophe theory, is described.

The structure of the semi-classical potential obtained within the SACM is not a simple polynomial with at most on simple factor of the type  $(1 + x^2)^n$ , but rather involved. Such complicated structures are common and the *catastrophe theory* provides us with an elegant method to tackle them.

## 3. The SACM

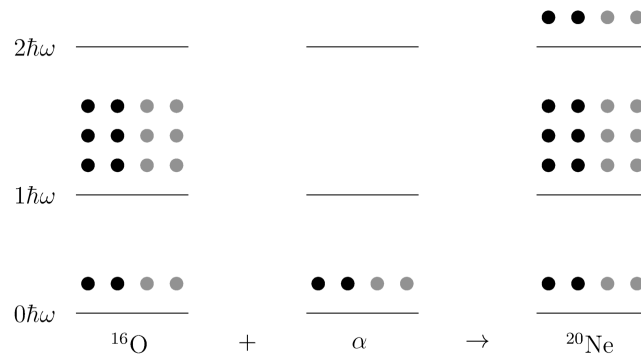
In the SACM [10, 11] the relative motion between clusters is described by the creation  $\pi_m^\dagger$  and annihilation  $\pi^m$  operators of the  $\pi$  bosons with angular momentum  $\ell = 1$ . (We use the notation of co- and contra-variant indices by lower and upper labels, respectively.) A cut-off  $N = n_\pi + n_\sigma$  is introduced, keeping  $N$  constant, by adding the creation  $\sigma^\dagger$  and annihilation  $\sigma$  of the  $\sigma$  bosons with angular momentum  $\ell = 0$ . Thus, the relative motion is described by a  $U_R(4)$  group structure.

The space used in this model is obtained by calculating the direct product of the  $SU(3)$  irreps  $(\lambda_k, \mu_k)$  of the clusters and the relative motion  $(n_\pi, 0)$  irrep, where  $n_\pi \geq n_0$  the number of  $\pi$  bosons is bounded from below satisfying the Wildermuth condition [5]. This product results in a linear combination of irreps, which is then compared with the fully antisymmetric shell model space, with the overlapping irreps used as the SACM space, thus observing the Pauli exclusion principle.



**Figure 1.** Critical manifold of the cusp catastrophe:  $V(x; a, b) = x^4/4 + ax^2/2 + bx$ . The green curve in the parameter space corresponds to the projection of the points where the tangent plane to the critical manifold is vertical, and is the bifurcation set separatrix.

In Fig. 2 the Wildermuth condition is illustrated and explained in the caption. It is a necessary condition and a violation leads automatically to a Pauli forbidden state.



**Figure 2.** The Wildermuth condition illustrated for the system  $^{16}\text{O} + \alpha \rightarrow ^{20}\text{Ne}$ . The left hand side show the distribution of nucleons of the two clusters within the shell model space and the right hand side gives the distribution in the united nucleus. From the left hand side we count 0 oscillation quanta for the  $\alpha$ -particle plus 12 quanta from the  $^{16}\text{O}$  nucleus, i.e., there are in total 12 oscillation quanta. The united nucleus has in total 20 oscillation quanta. Thus, in order to observe the *Pauli Exclusion Principle* the necessary condition is to add to the cluster system at least 8 quanta, the difference from the left to the right hand side of the figure. A smaller number of relative oscillation quanta automatically implies to put a nucleon in a lower, already occupied level. The black dots refer to protons and the gray ones to neutrons.

For the present time we will consider only systems of spherical clusters  $(\lambda_k, \mu_k) = (0, 0)$  to illustrate the procedure used, anticipating that when considering systems of deformed clusters

only makes the relations between the parameters of the model  $\{a, b, c, \xi\}$  and the parameters  $\{A, B, C, D\}$ , introduced below, more cumbersome, as will be shown in section 5.

The Hamiltonian considered consists of a linear combination of Casimir operators of the two dynamical symmetry group chains:  $SU_R(3)$  and  $SO_R(4)$ . The following simple form is considered:

$$\mathbf{H} = \mathbf{H}_{SU(3)} + \mathbf{H}_{SO(4)} \quad (1)$$

with

$$\mathbf{H}_{SU(3)} = \hbar\omega \mathbf{n}_\pi + (a - b\Delta \mathbf{n}_\pi) \mathbf{C}_2(\mathbf{n}_\pi, 0) + \xi \mathbf{L}^2 \quad (2)$$

$$\mathbf{H}_{SO(4)} = \frac{c}{4} [(\boldsymbol{\pi}^\dagger \cdot \boldsymbol{\pi}^\dagger) - (\boldsymbol{\sigma}^\dagger)^2] [(\boldsymbol{\pi} \cdot \boldsymbol{\pi}) - (\boldsymbol{\sigma})^2] \quad (3)$$

with  $\Delta \mathbf{n}_\pi$  is the number of shell excitations. When  $n_0$  is the minimal number of quanta needed to satisfy the Wildermuth condition and  $\mathbf{n}_\pi$  the number of relative oscillation quanta, then this  $\Delta \mathbf{n}_\pi$  is given by  $\mathbf{n}_\pi - n_0$ . The second order Casimir operator of  $SU_R(3)$  for the case of two spherical clusters is given by  $\mathbf{C}_2(\mathbf{n}_\pi, 0) = \mathbf{n}_\pi(\mathbf{n}_\pi + 3)$ .

The semi-classical potential is obtained as the expectation value  $V(\alpha) = \langle \alpha | \mathbf{H} | \alpha \rangle$  of this Hamiltonian in the basis of the coherent states defined as [9]

$$|\alpha\rangle = \frac{N!}{(N+n_0)!} \mathcal{N}_{N,n_0} \frac{d^{n_0}}{d\gamma^{n_0}} [\boldsymbol{\sigma}^\dagger + \gamma(\boldsymbol{\alpha}^* \cdot \boldsymbol{\pi}^\dagger)] |0\rangle \Big|_{\gamma=1} \quad (4)$$

where

$$\mathcal{N}_{N,n_0}^{-2} = \frac{(N!)^2}{(N+n_0)!} \frac{d^{n_0}}{d\gamma_1^{n_0}} \frac{d^{n_0}}{d\gamma_2^{n_0}} [1 + \gamma_1 \gamma_2 (\boldsymbol{\alpha}^* \cdot \boldsymbol{\alpha})]^{N+n_0} \Big|_{\gamma_1=\gamma_2=1} \quad (5)$$

is the normalization constant. It is convenient to define the arbitrary complex variables  $\alpha_m$  in terms of spherical coordinates:

$$\alpha_{\pm 1} = \frac{\alpha}{\sqrt{2}} e^{\pm i\phi} \sin \theta \quad (6)$$

$$\alpha_0 = \alpha \cos \theta. \quad (7)$$

The semi-classical potential is then obtained as

$$V = -b \left[ A \left( \alpha^2 \frac{F_{11}(\alpha^2)}{F_{00}(\alpha^2)} - n_0 \right) + (B + C \sin^2 2\theta) \left( \alpha^4 \frac{F_{22}(\alpha^2)}{F_{00}(\alpha^2)} - n_0(n_0 - 1) \right) + \left( \alpha^6 \frac{F_{33}(\alpha^2)}{F_{00}(\alpha^2)} - n_0(n_0 - 1)(n_0 - 2) \right) + D \cos 2\theta \alpha^2 \frac{F_{20}(\alpha^2)}{F_{00}(\alpha^2)} \right], \quad (8)$$

with functions  $F_{pq}(\alpha)$  defined in [12] and the  $c_i = \{A, B, C, D\}$  control parameters of the potential given in terms of the Hamiltonian parameters by

$$\begin{aligned} \bar{A} &= \hbar\omega + 4(a + b(n_0 - 1)) + 2\xi - \frac{c}{2}(N + n_0 - 1) \\ \bar{B} &= a + b(n_0 - 6) + \frac{c}{2} \\ \bar{C} &= \xi - \frac{c}{4} \\ \bar{D} &= \frac{c}{2} \\ \bar{X} &= -bX, \quad \text{with } X \in c_i. \end{aligned} \quad (9)$$

The procedure described works for any system of two spherical clusters, specified by the proper selection of  $n_0$  and  $N$ . As an example we consider the  $^{16}\text{O} + \alpha \rightarrow ^{20}\text{Ne}$  system, with  $n_0 = 8$  and  $N = 12$ , and by no means represents the real nucleus  $^{20}\text{Ne}$ , it will serve only to illustrate the structure of QPTs and to provide an  $n_0$ . The potential can then be written as

$$V(\alpha, \theta; c_i) = -b \frac{\alpha^2}{q_0(\alpha)} \left( A p_A(\alpha) + (B + C \sin^2 2\theta) p_B(\alpha) + D \cos 2\theta p_D(\alpha) + p_0(\alpha) \right), \quad (10)$$

with  $p_A(\alpha)$ ,  $p_B(\alpha)$ ,  $p_D(\alpha)$ ,  $p_0(\alpha)$  and  $q_0(\alpha)$  polynomials in even powers of  $\alpha$  and positive coefficients.

#### 4. Results

For our purposes, the basic concepts of catastrophe theory, that we used throughout the study of QPTs, are summarized in section 3 of [6]. There, the elementary cusp catastrophe is considered as an example and a *novel procedure* for the calculation of the Maxwell set is introduced. The Maxwell set is the subspace in parameter space where the value of the potential at two or more critical points is the same, e.g. the potential has two minima at the same depth,  $V(x_1; c_i) = V(x_2; c_i) = -V_0$ . The procedure developed to obtain the Maxwell set of a parameter dependent potential is based on the essence of catastrophe theory, which is the singular mapping of a *critical manifold*,  $\nabla V(x; c_i) = 0$ , to the parameter space  $(c_1, \dots, c_n)$ . In this case we construct what we call the *roots manifold*,  $V(x; c_i) + V_0 = 0$ , and calculate where the mapping to the parameter space is singular. This is justified because, whereas the singular mapping of the *critical manifold* happens at the coalescence of two critical points, the singular mapping of the *roots manifold* happens at the coalescence of two roots, thus creating a critical point  $x_c$  for which the value of the potential is at  $V(x_c; c_i) = -V_0$ . The singularity of the mapping is determined by the vanishing of the Jacobian determinant of the transformation, i.e. when the mapping is not invertible. For the present contribution we shall turn our attention to the potential (10) and specify the properties of QPTs found with the methods described above.

The semi-classical potential of the SACM depends on two variables  $(\alpha, \theta)$  and four parameters  $\{A, B, C, D\}$ . However, by applying the methods of catastrophe theory we found that there are only three essential parameters ( $\rho_2 = A, \rho_1 = B + C, D^2/C$ ) and in the  $\text{SU}_R(3)$  limit the essential parameter space is two dimensional ( $D = 0$ ). We are able, therefore, to begin in the  $(\rho_2, \rho_1)$  parameter space and treat the  $\text{SO}_R(4)$  dynamical symmetry ( $D \neq 0$ ) as an extension in the essential parameter space.

Evaluating the critical points of (10) in its two variables we obtain the following partial derivatives:

$$\begin{aligned} \frac{\partial V}{\partial \theta} &= -b \frac{2\alpha^2}{q_0(\alpha)} \left( C \sin 4\theta p_B(\alpha) - D \sin 2\theta p_D(\alpha) \right) \\ \frac{\partial V}{\partial \alpha} &= -b \frac{\alpha}{q_0^2(\alpha)} \left( A W_A(\alpha) + (B + C \sin^2 2\theta) W_B(\alpha) + D \cos 2\theta W_D(\alpha) + W_0(\alpha) \right), \end{aligned} \quad (11)$$

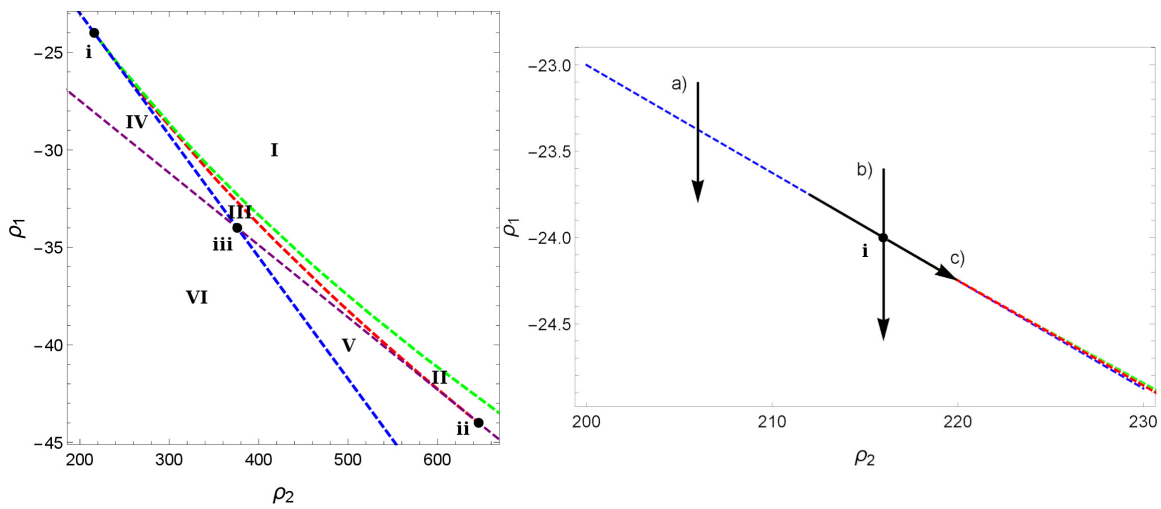
where we defined the function  $W_X(\alpha) = \alpha W(q_0, p_X) + 2q_0(\alpha) p_X(\alpha)$ , with  $W(f, g) = f(\alpha)g'(\alpha) - f'(\alpha)g(\alpha)$  the Wronskian determinant, and the prime indicates differentiation with respect to  $\alpha$ .

The angular  $\theta$  variable partial derivative vanishes when  $\cos 2\theta_c = D p_D(\alpha) / 2C p_B(\alpha)$ , which is  $\alpha$  dependent. This allows us to write the potential as a single variable function and in terms of the three essential parameters as:

$$V(\alpha; \rho_2, \rho_1, D^2/C) = -b \frac{\alpha^2}{q_0(\alpha)} \left[ \rho_2 p_A(\alpha) + \rho_1 p_B(\alpha) + \frac{D^2}{C} \frac{p_D^2(\alpha)}{4p_B(\alpha)} + p_0(\alpha) \right]. \quad (12)$$

Here we can restrict ourselves to the  $SU_R(3)$  limit by setting  $D = 0$ . Applying the methods of catastrophe theory, described in [6], we divided the parameter space  $(\rho_2, \rho_1)$  in six regions with the known separatrices, e.g. bifurcation set and Maxwell set.

In Fig. 3 the parameter space in the  $SU_R(3)$  limit is shown. The parameter space is divided in six regions where the potential has a similar qualitative behavior, and crossing the separatrices from one region to another signifies a QPT. The QPT is of first order when crossing the Maxwell set (red line). The QPT is of second order when crossing the blue line separatrix, illustrated in paths a) and b) in Fig. 3. A third order QPT occurs when crossing the so-called *germ* [7], represented as point i, along the blue line separatrix, as depicted in path c) in Fig. 3. In Fig. 4 we depict a potential whose qualitative behavior is representative for each of the six regions in the  $(\rho_2, \rho_1)$  parameter space.



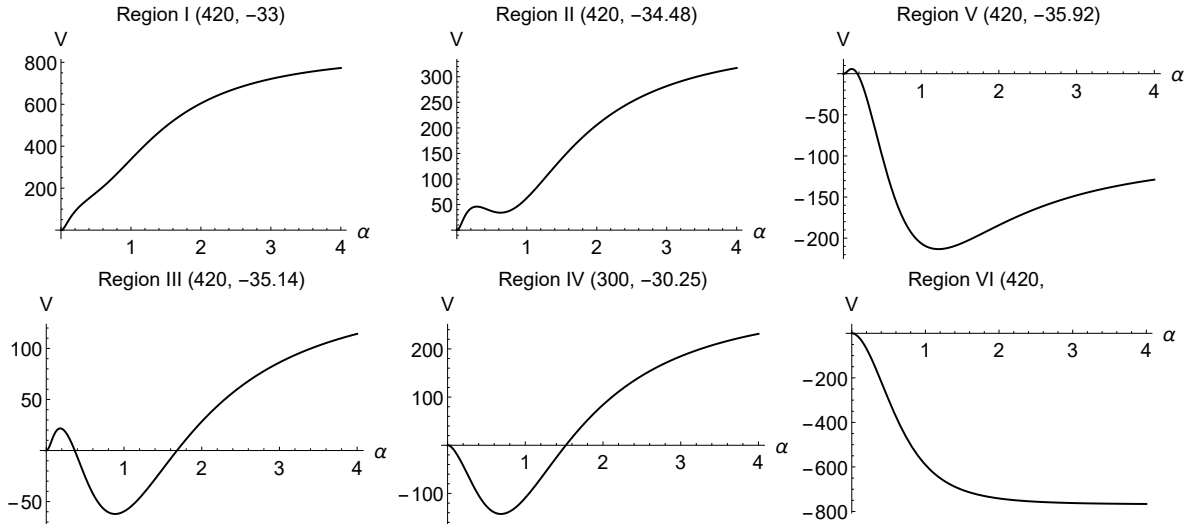
**Figure 3.** In the left is the parameter space  $(\rho_2, \rho_1)$  in the  $SU_R(3)$  limit (taken from [6]). The green dashed line is the bifurcation set and the red dashed line is the Maxwell set. The blue dashed line characterizes the critical point  $\alpha_0 = 0$ , i.e. it determines whether it is a maximum or a minimum. The purple dashed line divides the parameter space in two parts determining the asymptotic behavior, as  $\alpha \rightarrow \infty$ , of the potential, i.e. whether it is stable ( $V(\alpha \rightarrow \infty) > 0$ ) or unstable ( $V(\alpha \rightarrow \infty) < 0$ ). In the right is the parameter space zoomed in the vicinity of the *germ* and three paths taken. The order of the QPT of each path is: a) second order, b) second order, and c) third order.

## 5. Hamiltonian and parameter relations for systems of deformed clusters

When considering deformed clusters the second order Casimir operator  $C_2(\lambda, \mu)$  of  $SU_R(3)$  is given by

$$C_2(\lambda, \mu) = 2Q^2 + \frac{3}{4}L^2 \quad (13)$$

with  $Q = Q_C + Q_R$ , the total quadrupole operator, given as the sum of the cluster and relative quadrupole operators. The cluster quadrupole operator can be further divided as the sum of the two individual cluster quadrupole operators  $Q_C = Q_{C_1} + Q_{C_2}$ . Similarly, the square of the angular momentum operator can be written as  $L = (L_C + L_R)^2 = L_C^2 + L_R^2 + 2(L_C \cdot L_R)$ , where  $L_C$  corresponds to the cluster angular momentum, which can be further decomposed as



**Figure 4.** Example of representative potential of all six regions in  $(\rho_2, \rho_1)$  parameter space depicted in Fig. 3. Potentials in regions I through IV, above the purple line in parameter space, are stable; while potentials in regions V and VI, below the purple line, are unstable. The potential can have two minima, one at  $\alpha_0 = 0$  and other at  $\alpha_c > 0$ . The bifurcation set is crossed going from region I to region II, and then the critical point at  $\alpha_c > 0$  emerges. The Maxwell set is crossed going from region II to region III, and then the minimum at  $\alpha_c > 0$  is the global minimum.

$\mathbf{L}_C = \mathbf{L}_{C_1} + \mathbf{L}_{C_2}$ , the sum of the individual clusters angular momentum. Thus, the second order Casimir operator can be written as:

$$\mathbf{C}_2(\lambda, \mu) = \mathbf{C}_2(\lambda_C, \mu_C) + \mathbf{C}_2(\mathbf{n}_\pi, 0) + 4\mathbf{Q}_C \cdot \mathbf{Q}_R + \frac{3}{2}\mathbf{L}_C \cdot \mathbf{L}_R, \quad (14)$$

with  $(\lambda_C, \mu_C)$  the SU(3) irrep of the cluster system, and  $\mathbf{C}_2(\mathbf{n}_\pi, 0) = 2\mathbf{Q}_R^2 + 3\mathbf{L}_R^2/4$  is the second order Casimir operator of the relative motion.

Previously, when considering spherical clusters the Hamiltonian consisted only on relative motion operators, the expectation value of the Hamiltonian was performed in the basis of coherent states defined in (4). In the case of deformed cluster systems, the coherent states are changed to incorporate the internal cluster structure as done in [9].

The Hamiltonian considered for the case of deformed clusters is similar to the one defined in (1), the only change occurs in the  $\text{SU}_R(3)$  Hamiltonian, which is now considered to be

$$\mathbf{H}_{\text{SU}(3)} = \hbar\omega\mathbf{n}_\pi + (a - b\Delta\mathbf{n}_\pi)\mathbf{C}_2(\lambda, \mu) + (\bar{a} - \bar{b}\Delta\mathbf{n}_\pi)\mathbf{C}_2(\mathbf{n}_\pi, 0) + \xi\mathbf{L}^2. \quad (15)$$

With similar algebraic manipulations as the ones performed in the previous case, we obtain the semi-classical potential  $V \equiv V(\alpha, \theta; c_i)$  as

$$\begin{aligned} V = & -(b + \bar{b}) \left[ \left( A + E \cos \theta \right) \left( \alpha^2 \frac{F_{11}(\alpha)}{F_{00}(\alpha)} - n_0 \right) \right. \\ & + \left( B + F \cos \theta + C \sin^2 2\theta \right) \left( \alpha^4 \frac{F_{22}(\alpha)}{F_{00}(\alpha)} - n_0(n_0 - 1) \right) \\ & \left. + \left( \alpha^6 \frac{F_{33}(\alpha)}{F_{00}(\alpha)} - n_0(n_0 - 1)(n_0 - 2) \right) + D \cos \theta \alpha^2 \frac{F_{20}(\alpha)}{F_{00}(\alpha)} \right], \end{aligned} \quad (16)$$

with the control parameters  $c_i = \{A, B, C, D, E, F\}$  of the potential given by

$$\begin{aligned}
\bar{A} &= \hbar\omega - b\langle C_2(\lambda_C, \mu_C) \rangle + 4((a + \bar{a}) + (b + \bar{b})(n_0 - 1)) - \frac{c}{2}(N + n_0 - 1) \\
&\quad + (a + b(n_0 - 1))\Gamma_{12} + 2\xi \\
\bar{B} &= a + \bar{a} + (b + \bar{b})(n_0 - 6) + \frac{c}{2} - b\Gamma_{12} \\
\bar{C} &= \xi - \frac{c}{4} \\
\bar{D} &= \frac{c}{2} \\
\bar{E} &= 3(a + b(n_0 - 1))\Gamma_{12} \\
\bar{F} &= -3b\Gamma_{12} \\
\bar{X} &= -(b + \bar{b})X, \quad \text{with } X \in c_i,
\end{aligned} \tag{17}$$

with  $\Gamma_{12} = -(\Gamma^1 + \Gamma^2)/\sqrt{2}$  and  $\Gamma^k = \langle (\lambda_k, \mu_k) | Q_{C_k,0} | (\lambda_k, \mu_k) \rangle$ , the expectation value of  $m = 0$  component of the quadrupole operator of cluster  $k$  [12].

## 6. Conclusions

We presented a short review of the main results of previous work concerning QPTs in a non-trivial model [6]. We divided the essential parameter space of the SACM in distinct stability regions, where the family of potentials have similar qualitative behavior. This was done with the methods of catastrophe theory, and we described a novel procedure for obtaining the Maxwell set of a parameter dependent potential. We found that the order of the QPT may depend on the particular direction taken in the parameter space, as depicted in Fig. 3. Furthermore, the first steps in a line of research concerning systems of deformed clusters were presented. It was possible to obtain a semi-classical potential, and a more cumbersome relation between the interacting parameters and the control parameters was established, deserving further investigation.

Some of the future work to continue the line of research presented here is: Extend the results to systems of deformed clusters, modify the SACM to be able to include the analysis of systems of heavy nuclei, and the study of QPTs of excited states in the SACM using the cranking method.

## Acknowledgements

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