Phenomenological and semimicroscopic cluster models and their phase transitions

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Abstract. Two algebraic cluster models of nuclear structure which use the same Hamiltonian are explored: a Phenomenological Algebraic Cluster Model (PACM), and a Semi-microscopic Algebraic Cluster Model (SACM). The PACM does not incorporate the Pauli exclusion principle, while the SACM does. The Hamiltonian considered is an admixture of three dynamical symmetries; the $SU(3)$, $SO(4)$, and $SO(3)$, with weighting of each determined by parameters. The classical potential is constructed using coherent states, and the model Hilbert space of the SACM is constructed in such a way as to include all shell model states which correspond to the cluster structure of interest. Phase transitions and their orders are investigated for each model, and parameter phase diagrams are presented, wherein it is found that consideration of the Pauli principle has significant consequences. Also shown are fits of Hamiltonian parameters for a nucleus of 2 spherical clusters, when moving between the symmetry limits.

1. Introduction and formalism

To illustrate the significant effect of the Pauli principle in nuclear cluster studies, two algebraic nuclear cluster models are investigated: a Phenomenological Algebraic Cluster Model (PACM), and a Semi-microscopic Algebraic Cluster Model (SACM) [1, 2]. Both use a modified version of the vibron model [3] to describe relative motion, and the $SU(3)$ model of Elliott [4] for internal cluster structure. (The true vibron model describes clusters with the IBA [5, 6], and treats $\hbar \omega$ as a parameter, where here it is fixed by shell model considerations.) The difference between PACM and SACM is that the latter includes the Pauli exclusion principle for the combination of the nucleons of the two clusters.

It should be noted that here we deal not with nuclear molecules, such as the $\alpha + \alpha \rightarrow ^8\text{Be}$ system, which could be called ‘strong’ clusterisation. We deal rather with the ‘weak’ clusterisation of systems such as $^{16}\text{O}$, whose states can be considered to have some overlap with experimental basis states of the clusters $\alpha + ^{12}\text{C}$.

In both models, the relative motion degrees of freedom are oscillators in 3 dimensions, plus an additional auxiliary scalar boson, described by boson creation and annihilation operators:

$$\pi_m^\dagger, \pi_m, m = 0, \pm 1; \sigma^\dagger, \sigma.$$  \hspace{1cm} (1)

$\sigma$-bosons have no physical meaning, but define a cut-off for a conserved total number of bosons, $N = n_\pi + n_\sigma$. 

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In both PACM and SACM, the same Hamiltonian is used:

\[ \hat{H} = xy \hat{H}_{SU(3)} + y(1-x) \hat{H}_{SO(4)} + (1-y) \hat{H}_{SO(3)} \]  

(2)

where \( x \) and \( y \) are parameters ranging from 0 to 1, determining the strength of influence of different symmetries. In their most general form, the individual components are

\[ \hat{H}_{SU(3)} = \hbar \omega \hat{n}_\pi + a_C \hat{C}_2(\lambda_C, \mu_C) + (a - b \Delta \hat{n}_\pi) \hat{C}_2(\lambda, \mu) + \gamma \hat{L}_t^2 + t \hat{K}^2 \]  

(3)

\[ \hat{H}_{SO(4)} = a_C \hat{C}_2(\lambda_C, \mu_C) + a_C \hat{L}_C^2 + a_R^{(1)} \hat{L}_R^2 + \gamma \hat{L}_t^2 + C \left( (\hat{\pi}^\dagger \cdot \hat{\pi}^\dagger) - (\sigma^\dagger)^2 \right) \]  

(4)

and

\[ \hat{H}_{SO(3)} = \hbar \omega \hat{n}_\pi + a_C \hat{C}_2(\lambda_C, \mu_C) + a_C \hat{L}_C^2 + a_R^{(1)} \hat{L}_R^2 + \gamma \hat{L}_t^2 \]  

(5)

where \( \Delta \hat{n}_\pi = \hat{n}_\pi - n_0 \), with \( n_0 \) being the minimum number of quanta needed to satisfy the Pauli principle, as per the Wildermuth condition (see below). \( n_0 = 0 \) in the PACM. \( \Delta \hat{n}_\pi \) is included as without it, \( \hat{H} \sim \hat{n}_\pi - \hat{n}_\pi^2 \), with the latter dominating at high \( n_\pi \) [7]. The \( SO(3) \) limit is a special case of the \( SU(3) \), with only the \( \hbar \omega \hat{n}_\pi \) term plus couplings on the \( SO(3) \) level. \( \hat{K} \) is defined in [1, 2].

\( \hat{R} \) represents relative motion and \( \hat{C} \) denotes the internal structure of both clusters, the irreducible representations of the individual clusters being subsumed into irreducible representations of Elliott [4] in the relevant group chain, i.e. \( SU_C(3) \otimes SU_C(3) \otimes SU_R(3) \supset SU_C(3) \otimes SU_R(3) \) [see Eq. (3) of [8] for full chain used]. That is, the cluster number \( k \) : 1, 2 is within a definite \( SU_C(3) \) irrep \( (\lambda_k, \mu_k) \), and both are coupled to \( (\lambda_C, \mu_C) \). This is reflected on the operator level in Eq. (3) - (5). The generators of \( SU_C(3) \) are the sum of the generators of \( SU_C(3) \); for example, \( Q_{2m}^C = Q_{2m}^{C_1} + Q_{2m}^{C_2} \). Therefore, the second order Casimir operator is the sum of the Casimir operators of the individual clusters plus a coupling term.

Finally, \( (\lambda_C, \mu_C) \) is coupled with the relative motion irrep, \( (n_\pi, 0) \), yielding the total \( SU(3) \) irrep \( (\lambda, \mu) \). On the operator level, Eq. (3) - (5), this coupling is subsumed within the structure term. As an example of this, \( \hat{L}^2 = \hat{L}_R^2 + \hat{L}_C^2 + 2 \left( \hat{L}_R \cdot \hat{L}_C \right) \), reflecting the coupling of relative motion to the cluster irreps.

In the case of two spherical clusters, an example of which follows, \( (\lambda_k, \mu_k) = (0, 0) \), and thus \( (\lambda_C, \mu_C) = (0, 0) \), and so \( (\lambda, \mu) \) is \( (n_\pi, 0) \). All terms denoted with subscript \( C \) and fixed-body axis term, \( t \hat{K}^2 \), go to 0. For more details, see [1, 2].

In the study of phase transitions, it is necessary to define an intensive Hamiltonian, and one method is given in [9]. However, with a procedure based upon and constrained by the shell model, the situation is more subtle: it is not possible to divide the one-body interaction, \( \hbar \omega \hat{n}_\pi \), by \( N \), as this would lead, with increasing \( N \), to a zero inter-shell distance. Thus, as outlined below, in this work the coherent state parameter is related to the intercluster distance, which results in an \( N \)-independent expectation value of \( \hat{H} \). Thus, the result obtained is the same as in [9], but stemming from different arguments.

Consider again that we can write this one-body term as \( \hbar \omega (n_0 + \Delta \hat{n}_\pi) \), and that \( \hbar \omega n_0 \) can be included in the zero-point energy, \( \varepsilon_0 \), of [9] (though this is yet to be substantiated). Using coherent states and comparing the geometric quadrupole operator with the algebraic version of the same, it is shown in detail in [8] that

\[ \alpha \sim \frac{r - r_0}{\sqrt{N}} \]  

(6)

where \( r \) is the geometric inter-cluster distance and \( r_0 \sim \sqrt{n_0} \) (showing that the inclusion of the minimal inclusion of the Pauli principle automatically generates a minimal distance). This
\( \alpha \) is then used to form coherent states and thus a potential that does not go to infinity as \( N \) does. This can be seen in Eqs. (10) - (12) for PACM, where asymptotically, all \( N \) dependence vanishes (considering \( C \) to be a constant, which can be discarded, and \( c \) rescaled with \( N^{-1} \) dependency), and the same holds for SACM. A fuller account of this is in preparation.

This Hamiltonian is used to investigate phase transitions in clusterised nuclear matter, after defining a potential by forming diagonal matrix elements with coherent states [see Eq. (9) and (15)]. A first order phase transition is defined as a line of transition between which of a potential’s two wells is deepest. Crossing that line, the value of first derivative at the minima with respect to control parameters is not the same. I.e.,

\[
\frac{\partial V(\alpha_1)}{\partial P} \neq \frac{\partial V(\alpha_2)}{\partial P},
\]

where \( \alpha_1 \) and \( \alpha_2 \) are a minimum at the origin (spherical) with regards to one variable, and away from the origin (deformed) respectively. \( P \) represents control parameters.

A second order phase transition is a line of transition where, for our purposes, a deformed minimum in a potential becomes spherical. Crossing that line, the value of second derivative at the minima with respect to control parameters is not the same. I.e.,

\[
\frac{\partial^2 V(\alpha_1)}{\partial P^2} \neq \frac{\partial^2 V(\alpha_2)}{\partial P^2}.
\]

This idea generalises to higher order phase transitions [10, 11].

2. PACM

PACM makes no attempt to account for the Pauli principle, and its coherent states are

\[
|\alpha\rangle = \frac{1}{\sqrt{N!}} [\alpha \cdot \alpha]^{1/2} [\vec{\alpha} \cdot \vec{\pi}^\dagger]^{1/2} |0\rangle,
\]

where \( \alpha \) are variables representing a measure of inter-cluster distance. This coherent state, when applied to the Hamiltonian of Eq. (2), (3), (4) and (5), gives a potential of the form

\[
V = -N(N-1)(N-2)(xyb)\left\{A\frac{\alpha^4}{(1+\alpha^2)^2} - B\frac{\alpha^4}{(1+\alpha^2)^2} + \frac{\alpha^6}{(1+\alpha^2)^3}\right\} + C,
\]

where \( A, B \) and \( C \) are linearly independent functions of \( x, y, \) the Hamiltonian parameters and \( N, \)

\[
A = -\frac{xy[\hbar\omega + (a-b)(4 + (\Gamma_1 + \Gamma_2)) - b\mathcal{C}_2(\lambda_C, \mu_C)] - (1-x)y\epsilon(N-1) + (1-y)\hbar\omega}{xb(N-1)(N-2)},
\]

\[
B = \frac{x[a - 6b - b(\Gamma_1 + \Gamma_2)] + (1-x)c}{xb(N-2)},
\]

and

\[
C = xy\mathcal{C}_2(\lambda_C, \mu_C) + \frac{1}{4}(1-x)y\epsilon N(N-1).
\]

The central bracket of this, dependent on \( \alpha \) with parameters \( A \) and \( B \), is sufficient to investigate phase transitions, as shown in Fig. 1. In Region I, both a spherical and a deformed minimum exist, and the global minimum is deformed. In Region II, both a spherical and a deformed minimum exist, and the global minimum is spherical. In Region III only a spherical minimum exists, and in IV only a deformed. Solid lines are phase transitions, the horizontal being second order and the curved first order. Dashed lines are changes of region without phase
transition. Without third order terms, $\triangle \delta \pi$, $B$ is only defined for values less than zero, and thus only second order phase transitions exist, as in the model of [12].

Obtaining a fit to data for $\alpha^{16}O$, it was found that PACM is physically insufficient. When fixing parameters in the $SU(3)$ limit, considering the ground state band and restricting to even angular momentum the spectrum must start with $n_\pi = 0$, thus a $0^+$ state, and then $n_\pi = 2$, so a $0^+$ and a $2^+$ state. However, the $SU(3)$ Hamiltonian contains $\gamma L^2$, with $\gamma$ always positive, which forces $0_2^+$ to be lower in energy than the $2_1^+$. This defies the known data $E(2_1^+) = 1.634$ MeV and $E(0_2^+) = 8.7$ MeV.

Also, the $2_1^+$ state is of $1\hbar\omega$ excitation, where $\hbar\omega = 13.2$ MeV. Thus, the quadrupole-quadrupole interaction has to be unnaturally strong to locate this state at the experimental energy, 1.634 MeV. Such moves these higher-band states down to give the ground state band order $0^+_1, 2^+_1, 0^+_2$, but the $\langle n_\pi \rangle$ of these states are then 20, 20 and 0 respectively, meaning what should be $0^+_1$ is $0^+_2$, and the first two states are at the cut-off, and thus don’t converge.

Additionally, with different $n_\pi$ values for states in the ground state band, there are different $SU(3)$ structures in said band, so it is not a rotation band.

As one cannot use the $SU(3)$ limit for this nucleus as microscopic models guide one to, the $SO(4)$ is next examined. The $SO(4)$ limit is different to the $SU(3)$ as, in the former, a state is a mixture of many basis states in $SU(3)$. Here data can be fit well. However, when the arbitrary boson cut-off, $N$, is increased, the structure of the states change, implying that no convergence is reached. This is illustrated by the result [13]:

$$
\langle n_\pi \rangle = \frac{N - 1}{2}.
$$

(14)
This implies high shell excitations, and assuming that the two clusters are moving in a shell model mean field, one cannot make $\hbar \omega$ a parameter to overcome this and maintain that framework. Note also that any result based on an arbitrary cut-off cannot be physical.

3. SACM

SACM accounts for the Pauli principle by only considering states not forbidden in shell model calculations. For simple cluster systems, the minimal condition for achieving this is the Wildermuth condition [14], fully discussed in [1, 2, 8]. Then, the model space is obtained by comparing all possible irreps $(\lambda, \mu)$, contained in $(\lambda C_1, \mu C_1) \otimes (\lambda C_2, \mu C_2) \otimes (n_\pi, 0)$, with those of the shell model. Only those irreps appearing in shell model results are retained. In this microscopic approach, the Pauli principle is applied or not, and cannot be ‘tuned’. Note that $\hbar \omega$, which appears in the $SU(3)$ and $SO(3)$ Hamiltonians, must be a constant given by the shell model. It cannot, as in other models not guided by the shell model, be a parameter. The inclusion of $n_0$ from the Wildermuth condition yields the coherent state

$$|\alpha\rangle = N_{N,n_0} \frac{N!}{(N+n_0)!} \frac{d^{n_0}}{d\gamma^{n_0}} \left[ \hat{\sigma}^\dagger + \gamma (\alpha \cdot \hat{\pi}^\dagger) \right]^{N+n_0} |0\rangle , \quad (15)$$

where $N + n_0$ is now the total number of relative oscillation quanta, and the $\gamma$ parameter has to be set equal to 1 after differentiation. This leads to the potential

$$V = -xyb \left( A\alpha^2 \frac{F_{11}(\alpha^2)}{F_{00}(\alpha^2)} - B\alpha^4 \frac{F_{22}(\alpha^2)}{F_{00}(\alpha^2)} + \alpha^6 \frac{F_{22}(\alpha^2)}{F_{00}(\alpha^2)} - C\alpha^2 \frac{F_{20}^{N-2}(\alpha^2)}{F_{00}(\alpha^2)} \right) + D , \quad (16)$$
where $A$, $B$, $C$ and $D$ are linearly-independent parameters dependent on $x$, $y$, the Hamiltonian parameters, $n_0$ and $N$. The functions $F_{ij}$ are dependent on $\alpha$, $n_0$ and $N$. All are to be published elsewhere. Again, the $\alpha$-dependent component is sufficient for studying phase transitions. In all that follows, $n_0 = 8$ and $N = 12$, and a cross section of the phase space for these values and for $A = 10$ is shown in Fig. 2 (wherein red dots are points in Fig. 3). Increasing the number of bosons gives phase spaces with the same characteristics. Line types and regions are as in Fig. 1, with the addition of Region 0, in which no minima exist.

Note that this is a more complicated structure than the PACM, and contains an ‘end point’, beyond which the first order transition ceases to exist. This general structure is maintained at other values of $A$, making a flat plane of second order phase transition, and a curved plane of first order.

Fig. 3 gives a sample of energy functionals in different regions, the specific points being marked with lower-case letters in Fig. 2. From left to right, the first two panels show graphs either side of a phase transitions, points a) - d). The third shows a graph either side of the dotted line in the Region III of greater $B$, points e) and f), showing that while each have a barrier, one is bound as $\alpha \to \infty$, and the other is unbound. These tails are dependent on $N$, with the unbound approaching infinity and the bound negative infinity as $N \to \infty$. Thus, this region is unphysical. The Region III of lesser $B$, shown in the second panel, has no barrier, and is bound as $\alpha \to \infty$. The fourth panel shows a fully-bound potential with no minima from Region 0, point g).

4. SACM results
Using two spherical clusters simplifies the Hamiltonian. $\alpha+^{16}\text{O}$ is such a system, and is examined here. Coefficients for $SU(3)$ were fitted to give the best spectrum in that limit, then those remaining in the $SO(4)$ were fixed in that limit. Then, $x$ was varied with $y$ set to 1. In this way, the best fit for this nucleus is not sought, but phase transitions between symmetry limits are.

The left panel of Fig. 4 shows that a phase transition of second order occurs when $x = 0.6$. The plane is the second order phase transition surface, and the line is the system’s path as $x$ varies from 0 to 1, with $y = 1$. The right panel shows the ground state boson expectation, $\langle n_\pi \rangle$. The kinked line is from a geometrical mapping, and is dependent on the location in $\alpha$ of the deformed minimum. Beyond the phase transition at $x = 0.6$, there is no deformed minimum, and thus the boson expectation goes to the minimum of 8. The smooth line comes from numerical matrix diagonalisation, and has a mixing of states not seen in the geometrical mapping. Note that these results do not go to the cut-off, as was a problem for PACM.

As shown in Fig. 5, the order of low-lying $\alpha+^{16}\text{O}$ states in $^{20}\text{Ne}$ is recreated for all values of $x$, where $A$, $B$, $C$ and $D$ are linearly-independent parameters dependent on $x$, $y$, the Hamiltonian parameters, $n_0$ and $N$. The functions $F_{ij}$ are dependent on $\alpha$, $n_0$ and $N$. All are to be published elsewhere. Again, the $\alpha$-dependent component is sufficient for studying phase transitions. In all that follows, $n_0 = 8$ and $N = 12$, and a cross section of the phase space for these values and for $A = 10$ is shown in Fig. 2 (wherein red dots are points in Fig. 3). Increasing the number of bosons gives phase spaces with the same characteristics. Line types and regions are as in Fig. 1, with the addition of Region 0, in which no minima exist.

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and also that the $B(E2)$ value for the $2^+_1 - 0^+_1$ transition is well recreated when compared with experiment (dashed line), especially in the $SU(3)$ realistic for this nucleus. This is a numerical study, and while evidence of the phase transition is seen, it is not strongly so.

5. Conclusions

Differences appearing in the investigation of cluster models which do and do not obey the Pauli exclusion principle (SACM and PACM respectively) have been examined. The Hamiltonian used includes a modified vibron model [3] to describe relative motion, with $\hbar \omega$ fixed by shell model considerations, and the $SU(3)$ model of Elliott [4] for internal cluster structure, rather than the IBA [5, 6]. The Hamiltonian used interpolates between the $SU(3)$ limit, the $SO(4)$ limit, and the $SO(3)$ limit. In order to investigate phase transitions, when moving from one dynamical symmetry limit to another, the coherent state method was used. It was in the coherent states that the Pauli exclusion principle was first neglected and then applied. In the former case, the structure of the coherent state is the simplest.

In both cases, the phase space diagram was constructed in its most general form. Within the PACM only two relevant parameters appear, which in turn are functions of all the parameters of the model. Within the SACM one has three relevant parameters, which are again functions of all the interaction parameters of the theory. Both exhibit first- and second-order phase transitions, but the more complicated SACM phase space includes an ‘end line’. Potentials at a selection of illustrative points have been shown for the SACM.

The PACM has been shown to be unrealistic for modelling physical systems, while the SACM has been used successfully to model a physical nuclear system of two spherical clusters, $\alpha + ^{16}O$.
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