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**Rotational States Generated by SU(5) Dynamical Symmetry
with Constraints**

INTRODUCTION

The Generator Coordinate Method (GCM) proposed many years ago by Griffin, Hill and Wheeler [1] has been extensively used in many problems of nuclear physics e.g. see [2,3]. It is a fully quantum mechanical method that allows to investigate the nuclear collective motion by means of a very general ansatz for a trial function. It is a continuous superposition of the so-called generating functions $|q\rangle$ labelled by some number of real or complex parameters $q = \{q^1, q^2, \dots, q^r\}$, known as the generator coordinates. For every q the generator function is a vector in the many-body Hilbert space. The trial function is expressed by a multidimensional integral:

$$|\Psi\rangle = \int dq u(q) |q\rangle. \quad (1)$$

The standard variational principle leads to the very well known Griffin-Hill-Wheeler integral equations for the weight function $u(q)$ and collective energies. On the other hand, the GCM method can be treated as a kind of a projection technique that allows to construct a full collective space from a generator function [4]. In the present paper we follow the last idea.

For hot nuclei the ansatz (1) is not sufficient. It does not allow to introduce any temperature dependence into the formalism. The states (1) are pure states in the quantum mechanical sense but we need to generate the collective space from a given temperature, deformation and other characteristics dependent density matrix.

The way to this goal is proposed in this paper for the special case of rotational excitations (the method can be directly generalized to any arbitrary compact group of motion) extracted from a general quadrupole collective motion described by the dynamical symmetry group SU(5). This group of motion is the known symmetry group of the Bohr hamiltonian generated by the bilinear forms of quadrupole boson

operators. Using this simple model we will show a behaviour of rotational spectra of the five dimensional harmonic oscillator, the Bohr hamiltonian, simulating, in a simple way, spectra of some nuclei. Using the algebraical Gelfand-Najmark-Segal construction (GNS) [5,6] we construct a collective space generated from a fixed temperature dependent density matrix of our quadrupole bosons. The generator coordinates (the collective variables), that are needed for observation of the collective rotational motion, we introduce by means of the group $SO(3) \subset SU(5)$.

The method that we call the algebraic generator coordinate method (AGCM) allows for investigations of quantum systems with some constraints imposed by the symmetries. In this case we constrain the full quadrupole motion to the collective rotations only. The constraint, imposed by the rotational group $SO(3)$ contained in $SU(5)$, permits to obtain in a fully quantal way (without quantization) rotational states generated by an arbitrary $SU(5)$ generating hamiltonian. The procedure is state dependent and gives different spectra for different functionals of a state, (called also the metastates, in the sense of states defined in C^* algebra approach to quantum mechanics, see [7,5,6] and references therein). For the case when the metastate is defined by a density operator which is only dependent on the $SU(5)$ generating hamiltonian (e.g. a canonical density matrix) one can construct the rotational collective space and the corresponding rotational hamiltonian. The structure of the spectrum obtained by this procedure is dependent on the parameters in the metastate. For the canonical density operator one can observe a changing of rotational spectrum with the parameter corresponding to the quadrupole boson temperature of the system.

THE ROTATIONAL COLLECTIVE SPACE FOR $SU(5)$ DYNAMICAL SYMMETRY

In this case the method starts from the investigation of the formal integral operators

$$\int_G dg u(g) T(g) \quad (2)$$

where the functions $u \in L^2(G)$, $T(g)$ is the unitary representation of the group $G=SO(3) \subset SU(5)$ in a carrier space \mathcal{H} of unitary, totally symmetric representations of the group $SU(5)$ and dg is the Haar measure on G . The operators (2) form the $*$ -algebra, where the involution operation is defined as the hermitian conjugation. Now, having a given density operator ρ it is necessary to consider the eigenproblem for the generalized overlap operator \mathcal{N}_ρ :

$$(\mathcal{N}_\rho u_m)(g) \equiv \int_G dg' \langle \rho; T(g^{-1}g') \rangle u_m(g') = \Lambda(m) u_m(g), \quad (3)$$

where $\langle \rho; \cdot \rangle$ denotes the metastate, that for our purpose will be defined as the appropriate trace operation from the product of the density matrix ρ and the required operator S , i.e. $\langle \rho; S \rangle = Tr(\rho S)$. Because \mathcal{N}_ρ is well defined the hermitian compact operator its eigenfunctions span the whole space $L^2(G)$ and each element

of the algebra \mathcal{R} can be expressed as a series of the following basic elements

$$\int_G dg u_m(g) T(g). \quad (4)$$

By GNS construction [5,6] one can obtain the corresponding state space \mathcal{K} in which the algebra \mathcal{R} acts in a very natural way. This state space \mathcal{K} is a generalization of the collective state space of the standard GCM (Generator Coordinate Method) procedure. Both construction AGCM and GCM are equivalent when a metastate in the first method is defined by the mean value, i.e. $\rho = |\phi\rangle\langle\phi|$:

$$\langle\phi; T(g)\rangle = \langle\phi|T(g)|\phi\rangle, \quad (5)$$

where $T(g)|\phi\rangle$ is a generator function for GCM approach. For the metastate defined by a quantum mechanical density operator there is no corresponding standard GCM construction. In this sense AGCM is a generalization of GCM.

The elements of the states space \mathcal{K} are in fact classes of equivalent algebra elements (denoted in further text by $\text{cl}()$) with respect to the functional $\langle\rho; \cdot\rangle$: each class contain the elements which differ from each other on a null element (i.e. an element of the algebra which is indistinguishable by the state functional from zero element of the algebra). Those null elements furnish the subalgebra generated by the operators (4) related to all m 's for that the eigenvalues $\Lambda(m)$ of the overlap operator \mathcal{N}_ρ are equal to zero, i.e. $\Lambda(m) = 0$. This means that the space \mathcal{K} is spanned by the following basic vectors:

$$e_m \equiv \frac{1}{\sqrt{\Lambda(m)}} \text{cl}_\mathcal{K}(P_m), \text{ for } \Lambda(m) \neq 0. \quad (6)$$

The scalar product in \mathcal{K} is defined now as:

$$\langle\text{cl}_\mathcal{K}(S) | \text{cl}_\mathcal{K}(R)\rangle \equiv \langle\rho; S^+ R\rangle, \quad (7)$$

where S and R are elements of the group algebra \mathcal{R} . This way (after the standard procedure to complete the pre-Hilbert space defined above) one obtains the states space \mathcal{K} for a collective motion generated by the group G . In addition the metastate constrains the motion to the one that can be obtained by excitations of the density operator defining $\langle\rho; \cdot\rangle$.

For the totally symmetric irreducible representations of the group SU(5) the carrier space \mathcal{H} is spanned by the states labelled by five quantum numbers $|N\nu\mathbf{x}LM\rangle$, where N is the number of quadrupole bosons, ν denotes the seniority number, \mathbf{x} can be interpreted as a maximal number of boson triplets coupled to zero angular momentum, and L and M are the usual angular momentum quantum numbers [8].

The state functional (the metastate) is chosen in the form of trace in the space \mathcal{H} from the product of the density operator ρ and a needed operator S :

$$\langle\rho; S\rangle = \text{Tr}_{\text{SU}(5)}(S \cdot \rho) = \sum_{N\nu\mathbf{x}LM} \langle N\nu\mathbf{x}LM | S \cdot \rho | N\nu\mathbf{x}LM \rangle. \quad (8)$$

Let us denote by $\rho(N\nu\mathbf{x}LM) = (N\nu\mathbf{x}LM|\rho|N\nu\mathbf{x}LM)$ and assume that the density operator ρ is axially symmetric, i.e. it is invariant under rotations around the z -axis. For simplicity we consider only a class of hamiltonians H that are diagonal in the basis $|N\nu\mathbf{x}LM\rangle$ i.e.

$$H|N\nu\mathbf{x}LM\rangle = E(N\nu\mathbf{x}LM)|N\nu\mathbf{x}LM\rangle. \quad (9)$$

This case corresponds e.g. to the standard five dimensional harmonic oscillator and to so-called vibrational limit of the IBM model [9].

The action of the overlap operator \mathcal{N} can be now written:

$$\begin{aligned} (\mathcal{N}_\rho u)(\Omega) &= \int_{\text{SO}(3)} d\Omega' \text{Tr}_{\text{SU}(5)}(R_{\text{SO}(3)}(\Omega^{-1}\Omega') \cdot \rho) u(\Omega') = \\ &= \sum_{N\nu\mathbf{x}LM} \int_{\text{SO}(3)} d\Omega' \langle N\nu\mathbf{x}LM|\rho \cdot R_{\text{SO}(3)}(\Omega')|N\nu\mathbf{x}LM\rangle u(\Omega\Omega') = \\ &= \sum_{N\nu\mathbf{x}LM} \rho(N\nu\mathbf{x}LM) \int_{\text{SO}(3)} d\Omega' D_{MM}^L(\Omega') u(\Omega\Omega'), \end{aligned} \quad (10)$$

where $R_{\text{SO}(3)}(\Omega)$ is the rotational operator with the Euler angles Ω , $\Omega\Omega'$ denotes the Euler angles corresponding to the composition of two rotations $R_{\text{SO}(3)}(\Omega)$ and $R_{\text{SO}(3)}(\Omega')$. After some straightforward calculations, making use of invariance property of the Haar measure the eigenvalues and eigenfunctions of the overlap operator can be found in the analytical form:

$$\begin{aligned} \Lambda(LK) &= \sum_{N\nu\mathbf{x}} \frac{\rho(N\nu\mathbf{x}K)}{2L+1} \\ u_{LMK}(\Omega) &= \sqrt{2L+1} D_{MK}^{L*}(\Omega). \end{aligned} \quad (11)$$

By insertion of eqs. (11) into (6) one obtains the basis e_{MK}^L for the state dependent collective rotational space projected from the full $\text{SU}(5)$ carrier space of totally symmetric representations including possible equivalent representations. Now one can calculate the matrix elements of the hamiltonian H :

$$H_{(L'M'K')(LMK)} = (e_{M'K'}^{L'}|e_{MK}^L) = \frac{1}{\sqrt{\Lambda(L'K')\Lambda(LK)}} (\rho; P_{M'K'}^{L'} \cdot H \cdot P_{MK}^L). \quad (12)$$

In our case of hamiltonians diagonal in the group chain $\text{SU}(5) \supset \text{SO}(5) \supset \text{SO}(3)$ the formula simplifies:

$$H_{(L'M'K')(LMK)} = \frac{\partial_{L'L} \partial_{M'M} \partial_{K'K}}{(2L+1)\Lambda(LK)} \sum_{N\nu\mathbf{x}} E(N\nu\mathbf{x}LM) \rho(N\nu\mathbf{x}LK), \quad (13)$$

and for the rotational energy one gets the expression:

$$\mathcal{E}_{\text{rot}}(LMK) = \frac{\sum_{N\nu\mathbf{x}} E(N\nu\mathbf{x}LM) \rho(N\nu\mathbf{x}LK)}{\sum_{N\nu\mathbf{x}} \rho(N\nu\mathbf{x}LK)}. \quad (14)$$

The formula (14) describes, in general, rotation K -bands and M dependent energies for hamiltonians containing the third component angular momentum operator L_z . The K -bands can be not degenerated in K for the density operators dependent on L_z .

THE TEMPERATURE DEPENDENT FIVE DIMENSIONAL HARMONIC OSCILLATOR

In the nuclear physics the 5-dimensional harmonic oscillator simulates main feature of the collective quadupole motion. We consider here a temperature dependent rotational motion within the SU(5) model. To this goal we choose the density operator in the canonical form:

$$\rho = Z^{-1} \exp(-\beta H_{\text{gen}}), \quad \beta = \frac{1}{kT}, \quad Z = \text{Tr}_{\text{SU}(5)}(\rho), \quad (15)$$

where the generating hamiltonian we choose as the 5-D harmonic oscillator hamiltonian $H = \hbar\omega(N + 5/2)$ plus any function of L^2 and L_o operators:

$$H_{\text{gen}} = \hbar\omega(N + 5/2) + f(L^2, L_o) \equiv \hbar\omega N + f'(L^2, L_o). \quad (16)$$

The selection rules for the quantum numbers are the following [8,9]:

$$\begin{aligned} N &= 0, 1, 2, \dots, \infty, \\ v &= N, N-2, N-4, \dots, 0 \text{ or } 1, \\ 0 &\leq x \leq v/3, \\ v-3x &\leq L \leq 2(v-3x), \\ L &\neq 2(v-3x)-1. \end{aligned}$$

The multiplicities s_{NL} of the states for given N and L , and all possible v and x , are given in the Appendix. There are listed the multiplicities s_{NL} for $L < 21$ and $N < 31$. Using these coefficients the rotational energies can be rewritten as:

$$\begin{aligned} \mathcal{E}_{\text{rot}}(0)_{LK} &= \frac{\sum_N s_{NL} (\hbar\omega N + 5/2\hbar\omega) \exp[-\beta\hbar\omega N - \beta f'(LK)]}{\sum_N s_{NL} \exp[-\beta\hbar\omega N - \beta f'(LK)]} = \\ &= -\hbar\omega \frac{\partial}{\partial a} \left[\frac{\sum_N s_{NL} \exp(-aN)}{\sum_N s_{NL} \exp(-aN)} \right] + \frac{5}{2} \hbar\omega, \end{aligned} \quad (17)$$

where $a \equiv \beta\hbar\omega$. This expression describes the temperature dependent rotational spectrum projected out of the considered harmonic oscillator. This spectrum, as it could be expected, has no special regularities typical for rotators because of strong coupling between the rotational and vibrational degrees of freedom in H . However, one needs to remember that the group $G = \text{SO}(3)$ constrains the hamiltonian H and reduces degrees of freedom of the system to three angles of rotations only. To some extent it is a quantum analog of a separation of the rotational and vibrational energy in the Bohr hamiltonian [10]. The results are different because in the Bohr model case the separation is performed first and then

the obtained classical hamiltonian is quantized; in our case the whole quantum spectrum is analysed in terms of different motions. We check if a given energy level survives after reduction of the state space to the required type of motion. In the formula (17) one can also notice that in the generating hamiltonian a dependence of $f'(L^2, L_0)$ is irrelevant. This means that adding to H_{gen} a pure rotational hamiltonian changes neither the collective space nor eigenenergies. This type of 'gauge' symmetry of the generating hamiltonian is an interesting feature of the formalism and probably is of a general nature. This problem requires further investigations.

In the Appendix there are shown the analytical formulas for the rotational energy \mathcal{E}_{rot} for $L < 8$. One can notice that for each temperature the spectrum corresponding to odd angular momenta is shifted by a constant value in respect to even angular momenta states, namely:

$$\mathcal{E}_{\text{rot}}(L+3) - \mathcal{E}_{\text{rot}}(L) = 3\hbar\omega. \quad (18)$$

In the vibrational nuclei like ^{106}Pd the energy of the first 3^+ state is just $3\hbar\omega$ above the ground state corresponding to $L = 0$. The relation (18) suggests that also for $T > 0$ case, i.e. for the hot quadrupole boson gas this pair of states should have the same splitting.

Fig. 1 shows the temperature dependent rotational spectrum relative to $L = 0$, i.e. $\mathcal{E}_{\text{rot}}(0) = 0$ for each temperature T . One can see that instead of three metastate parameters taken primarily: T , ω and an arbitrary function $f'(LM)$ we obtain only one parameter dependence: the function $f'(LM)$ vanishes and ω and T are coupled together so that ω is in fact only the scaling factor of the temperature T . In addition, the energy is degenerated in K because there is no dependence of ρ or the hamiltonian of the system on a third component angular momentum operator.

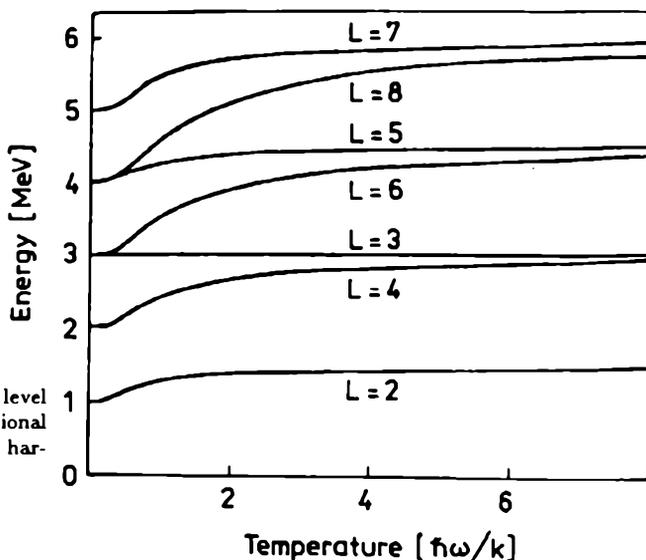


Fig. 1. The relative to $L = 0$ level temperature dependent rotational spectrum of five-dimensional harmonic oscillator is plotted

The $T = 0$ case is of great interest here. The spectrum for zero temperature is obtained as the limit of the expression (17) calculated with $T \rightarrow 0^+$.

Direct use of the density operator ρ for $T = 0$ to generate the rotational spectrum of the 5-D harmonic oscillator gives no effect because this state is the rotationally invariant state vector with the total angular momentum $L = 0$ and by rotations one can obtain only this ground state itself. This analysis shows that using of more general metastates than those that are determined by the pure states allows for generation of the rotational spectra even for undeformed nuclei. For 5-D h.o. with $T = 0$ the SO(3) spectrum is described by two simple sequences:

$$\mathcal{E}_{\text{rot}}(L, T = 0) = \begin{cases} \hbar\omega(\frac{1}{2}L + 5/2); L = 0, 2, 4, \dots \\ \hbar\omega(\frac{1}{2}(L + 3) + 5/2); L = 3, 5, 7, \dots \end{cases} \quad (19)$$

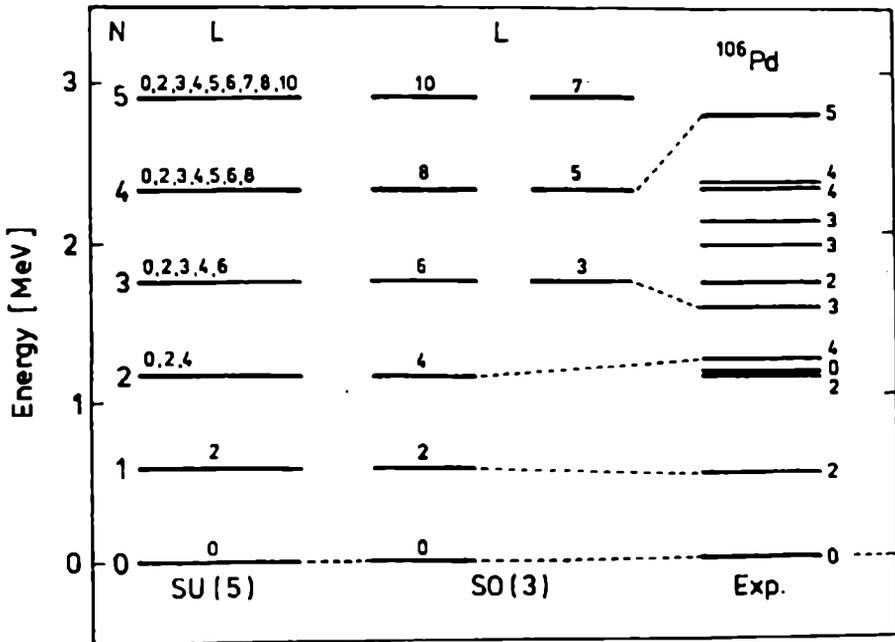


Fig. 2. In the figure the separation of the SO(3) (rotational) spectrum, $T = 0$, from the 5-D harmonic oscillator with comparison to the experimental spectrum of ^{106}Pd , $\hbar\omega = 0.58$ MeV, is shown

In Fig. 2 there are shown SU(5) and SO(3) spectra for the boson temperature $T = 0$. The states that survive after reduction of the full harmonic oscillator to only 3 rotational degrees of freedom consist of the boson configurations having the lowest number of bosons that can be coupled to required angular momenta, i.e. for an even angular momentum $L = 2N$, $N = v$ and $x = 0$ and for an odd one $L = 2N - 3$ with the same relations for the seniority number v and the maximal number of boson triplets x . The rotational spectrum for $T = 0$ is equidistant like vibrational one. For $T > 0$ one can observe doublets $(L, L-1)$ with even $L = 0, 2, 4, \dots$

These doublets are also practically equidistant. The levels of odd L are degenerated with levels of $L + 3$ for $T = 0$ and with $L + 1$ for $T = \infty$. For $T \neq 0$ each level is $(2L + 1)^2$ times degenerated, for $T = 0$ the levels with $L \geq 3$ have degeneracy two times higher.

We mentioned above that for $T = 0$ the levels which survive after blocking other degrees of freedom than those allowing for the rotational motion have the possible lowest energy for the given angular momentum. The question arises what the structure of these rotational levels for $T \neq 0$ is. This problem leads to another property of the AGCM formalism that allows to represent the state vectors obtained in one collective space into another collective space which can be constructed from the algebra of the operators (2) but with $G = SU(5)$ and eventually different metastates. This feature of the formalism enables to consider the phenomena whose description, in general, requires the variable state spaces. Returning to our problem one can immediately see that the solution of the overlap operator eigenquation (3) for $G = SU(5)$ can be written thus:

$$\begin{aligned} \Lambda_{SU(5)}(Nv'x'L'K) &= \frac{\rho(Nv'x'L'K)}{\dim_{SU(5)}[N]} \\ w_{N,vxLM,v'x'L'K}(g) &= \sqrt{\dim_{SU(5)}[N]} D_{vxLM,v'x'L'K}^N(g), \end{aligned} \quad (20)$$

where D-function denote the matrix elements of the irreducible representations of the group $SU(5)$. Using the eigenfunctions (20) the corresponding collective space of the 5-D h.o. is spanned by the basic vectors (6) denoted now for the given boson temperature T as:

$$e_{vxLM,v'x'L'K}^N(T). \quad (21)$$

The rotational states $e_{MK}^L(T)$ for the temperature T can be expanded in the basic vectors (21). After some algebra one can get that the corresponding rotational vectors within the five dimensional harmonic oscillator space are given by the formula:

$$\begin{aligned} e_{MK}^L(T) &\rightarrow e_{LMK}^{SU(5)}(T) = \\ &= \left\{ \sum_{Nvx} \rho(NvxLK; T) \right\}^{-1/2} \sum_{Nvx} \rho(NvxLK; T)^{1/2} e_{vxLM,v'x'L'K}^N(T). \end{aligned} \quad (22)$$

The energy calculated with the states (22) is given by the expression (14). On the other hand the eigenenergies of the 5-D h.o. within the space spanned by the vectors (21) are obviously independent of the temperature and are given by the usual formula $\hbar\omega(N + 5/2)$. This allows to interpret the squared expansion coefficients in eq. (22) as the occupation probabilities of the harmonic oscillator states:

$$p_{vxLMK}^N(T) = \frac{\rho(NvxLK; T)}{\sum_{Nvx} \rho(NvxLK; T)}. \quad (23)$$

To exemplify a typical behaviour of the occupation probabilities one can obtain the analytical formula from the expression (23) for the special case of the angular momentum $L = 2$ (with the help of eq. (A2, Appendix)):

$$P_{v,\epsilon 2MK}^N(T) = \frac{y^{N-1}(1-y^3)^2}{1+y+y^2} \quad \text{for } N > 0. \quad (24)$$

where $y = \exp(\hbar\omega/kT)$. In Fig. 3 there is plotted the occupation probability function (24). One can notice that for the lowest allowed shell, i.e. for $N = 1$, for $T = 0$ the function (24) is equal to 1 and it is a decreasing function with T while other energy levels at this moment are unoccupied and their occupation probabilities vanish. The probability functions (24) for $N > 1$ have a characteristic shape with a single maximum.

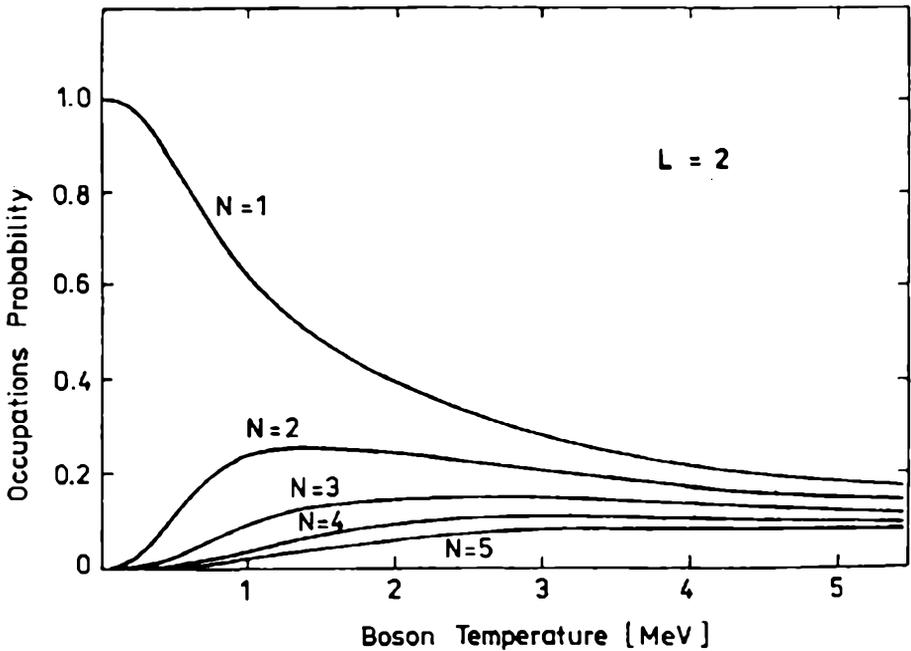


Fig. 3. In the figure some examples of the occupation probability functions for $L = 2$ and different shells are plotted

The above analysis suggests the idea of the spontaneous thermal transitions. The transitions can go along the line with the same angular momentum from the rotational state with higher temperature to the lower one. These thermal transitions should be similar to the nuclear giant resonances. The 5-D harmonic oscillator model is too schematic to perform more realistic considerations that will be a topic of further work.

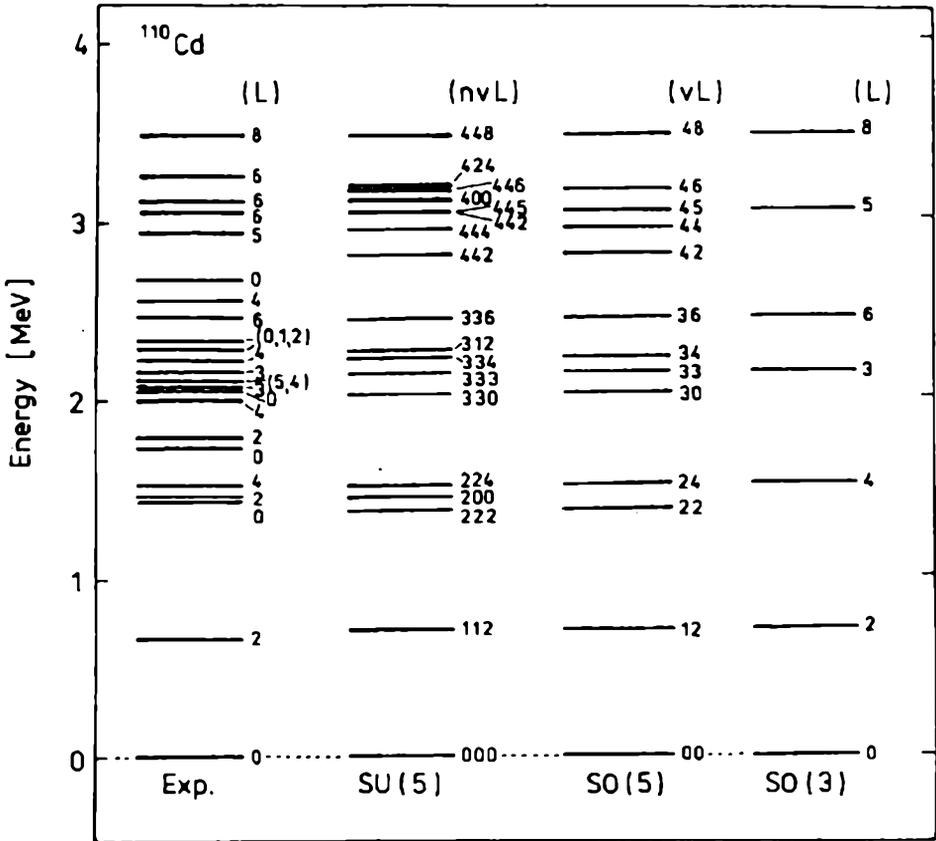


Fig. 4. The AGCM group theoretical classification of the spectrum for ^{110}Cd . The vibrational limit of the IBM model hamiltonian has been used [9] (not described in the text)

CONCLUSION

In this paper, we have demonstrated some basic results of using of the AGCM method for the construction of a collective subdynamics in terms of motions generated by certain groups of motions. Explicitly we have done this for rotational motion generated from the five dimensional harmonic oscillator. These preliminary results indicate the fact that spectra and in general spaces of quantum states of constrained systems are not constant and can change with some external parameters, e.g. with deformation or temperature of the system. On the other hand the AGCM approach allows for a new type of group theoretical classifications of the collective spectra: one can investigate invariance of given collective excitations in the degrees of freedom reduction procedure to the required type of motion. Here we have considered only the rotational subgroup of the group $SU(5)$, but also the subgroup $SO(5)$ is of great importance. The idea of transitions between the

collective spaces corresponding to different deformations or temperatures requires also further investigation within more realistic models than presented in the paper.

APPENDIX

The multiplicity s_{NL} of the states $|N\ell LM\rangle$ for given N and L :

$L \setminus N$	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20		
0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0

The calculate the energy one has to find the value of the formula:

$$\Theta = \sum_{N=0}^{\infty} s_{NL} e^{-aN}. \tag{A1}$$

To do that one needs to find a regularity in s_{NL} for each L separately and use the well-known formulae:

$$\sum_{N=0}^{\infty} e^{-aN} = \frac{1}{1 - e^{-a}} \text{ and } \sum_{N=0}^{\infty} N e^{-aN} = \frac{e^{-a}}{(1 - e^{-a})^2}.$$

We will demonstrate it for one of the simplest cases, $L = 2$, where s_{NL} form a series:

N	1	2	3	4	5	6	7	8	9	...
s_{NL}	0	1	1	1	2	2	2	3	3	3...

We proceed:

$$\begin{aligned} \Theta_{L=2} &= \sum_{N=0}^{\infty} s_{N2} e^{-aN} = \sum_{s=0}^{\infty} s e^{-a(3s-1)} + \sum_{s=0}^{\infty} s e^{-a(3s-2)} + \sum_{s=0}^{\infty} s e^{-3as} = \\ &= \sum_{s=0}^{\infty} s e^{-3as} (1 + e^a + e^{2a}) = \frac{e^{-a} + e^{-2a} + e^{-3a}}{(1 - e^{-3a})^2}. \end{aligned} \tag{A2}$$

After some transformations we get the analytical formulae for the rotational energies. For simplicity we use the abbreviation:

$$x = \exp\left(\frac{\hbar\omega}{kT}\right).$$

For the lowest angular momenta from $L = 0$ to 8 we find in the units $\hbar\omega$:

$$\begin{aligned} \mathcal{E}_{\text{rot}}(0) &= \frac{5 + 5x + 4x^2 + 5x^3 + 5x^4}{2(x-1)(1+x)(1+x+x^2)} \\ \mathcal{E}_{\text{rot}}(2) &= \frac{1 + 2x + 2x^2 + 7x^3}{2(x-1)(1+x+x^2)} \\ \mathcal{E}_{\text{rot}}(3) &= \frac{-1 - x + 4x^2 + 11x^3 + 11x^4}{2(x-1)(x+1)(1+x+x^2)} \\ \mathcal{E}_{\text{rot}}(4) &= \frac{-3 + 2x + 9x^2}{2(x-1)(x+1)} \\ \mathcal{E}_{\text{rot}}(5) &= \frac{-5 + 2x + 2x^2 + 13x^3}{2(x-1)(1+x+x^2)} \\ \mathcal{E}_{\text{rot}}(6) &= \frac{-7 + 2x - x^2 + 17x^3 + 2x^4 + 11x^5}{2(x-1)(x+1)(1+x+x^2)} \\ \mathcal{E}_{\text{rot}}(7) &= \frac{-9 + 2x + 15x^2}{2(x-1)(x+1)} \\ \mathcal{E}_{\text{rot}}(8) &= \frac{-11 - 20x - 12x^2 + 13x^3 + 36x^4 + 37x^5 + 36x^6 + 28x^7 + 13x^8}{2(x-1)(x+1)(1+x+x^2)(1+x+x^2+x^3+x^4)} \end{aligned} \quad (\text{A3})$$

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