The algebraic generator coordinate method as the constrained quantum mechanics

1992 J. Phys. A: Math. Gen. 25 4613

(http://iopscience.iop.org/0305-4470/25/17/020)

J. Phys. A: Math. Gen. 25 (1992) 4613-4624. Printed in the UK

The algebraic generator coordinate method as the constrained quantum mechanics*

A Boguszt and A Góźdź‡

Institute of Physics, M Curie-Skłodowska University, pl. M Curie-Skłodowskiej 1, 20-031 Lublin, Poland

Received 8 November 1991, in final form 13 March 1992

Abstract. In the paper, the principles of the algebraic generator coordinate method are presented. The construction of the collective space for a many-body system described by a density matrix is shown.

1. Introduction

The generator coordinate method (GCM) originally founded by Griffin *et al* [1] has been used successfully in many problems of nuclear physics, e.g. see [2]. It is a fully quantum mechanical method that allows construction of some spaces of states of 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 a certain number of real or complex parameters $q=\{q^1, q^2, \ldots, q^r\}$, the so-called 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

$$|\Psi\rangle = \int \mathrm{d}q\, u(q)|q\rangle. \tag{1}$$

The variational principle for the expectation value of the total many-body Hamiltonian H leads to the very well known Griffin-Hill-Wheeler integral equations for the weight function $u(q)$. There are many useful approximations to the exact method [2]. Here we want to mention only one of the more elegant ones called the Gaussian overlap approximation where it is possible to obtain directly a collective Hamiltonian in the form of the usual second-order differential operator for collective energy plus a collective potential corrected by the zero-point energy [3]. On the other hand, the GCM method can be treated as a kind of a projection technique that allows construction of a full collective space from a generator function [4].

The states (1) are pure states in the quantum mechanical sense. For many cases where a statistical approach is required the ansatz (1) is not sufficient and does not provide the appropriate formalism. One needs to extend the GCM approach to the mixed states generated from a given density matrix. The way to this goal is proposed

* Work supported by the Polish Ministry of Education, grant no. II.1.1.P/04/399.

† E-mail: BOGUSZ AT PLUMCS11.BITNET

‡ E-mail: GOZDZ AT PLUMCS11.BITNET

0305-4470/92/174613+12$04.50

in this paper. We construct a collective space generated from a fixed density matrix of the system under consideration. We introduce the generator coordinates (the collective variables) by means of the appropriate group of motions, a compact Lie group as, for example, in [5] for pure states. What we call the group of motions defines the possible types of excitations in the physical system, in many cases it corresponds to the dynamical symmetries. The case of a compact group is more elementary and does not require very refined algebraical and analytical methods. This allows us to show more clearly the main features of the formalism and give a physical interpretation to it. Extension to the non-compact case is currently in progress. Because of the extended use of algebraical methods we call the proposed approach the algebraic generator coordinate method (AGCM).

2. A construction of a collective space

In this section we describe the main steps that are needed to construct the collective space generated by a density operator and a given group of motions. Most of the required mathematical details to support the physical intuition are given in the appendix, and the practical way of using the formalism in the main text. We follow the basic idea of the GNS construction [6, 7] that was used intensively in the algebraical approach to statistical classical and quantum mechanics. The main object in this formalism is an algebra with involution and the space of functionals on it. These functionals are called the metastates of the system [8].

For a given (usually approximate) density operator ρ of the physical many-body system described in the appropriate many-body Hilbert space $\mathcal{H}$ we choose a symmetric *-algebra $\mathcal{A}(G)$ [9-11] of all operators $T(g)$, where $g \in G$ and G is a compact group of motions, furnishing a unitary operator representation of the group G in the carrier space $\mathcal{H}$. More precisely speaking this algebra is the smallest C^* algebra of operators in $\mathcal{H}$ containing the operator representation T. On the algebra $\mathcal{A}(G)$ one can define a natural positively defined functional (the metastate) generated by the density operator ρ as follows:

$$\langle \rho; S\rangle = \mathrm{Tr}(\rho S) \qquad \text{where } S \in \mathcal{A}(G). \tag{2}$$

The density operator is normalized in the standard way to unity. One can notice here that the functional (2) satisfies the very well known Cauchy–Schwartz inequality

$$|\langle \rho; S^+R\rangle|^2 \leq \langle \rho; S^+S\rangle\langle \rho; R^+R\rangle \qquad \text{for all } S, R \in \mathcal{A}(G). \tag{3}$$

Particularly, from the expression (3) one can see that the function $\langle \rho; T(g)\rangle$ is bounded, namely

$$|\langle \rho; T(g)\rangle| \leq 1 \qquad \text{for all } g \in G. \tag{4}$$

This property is essential for mathematical proofs in further considerations.

Following the idea of the GCM method one can now postulate a generalization of the ansatz (1) introducing the algebra consisting of the following elements:

$$\int_G \mathrm{d}g\, u(g) T(g) \tag{5}$$

where dg means the invariant Haar measure on G and the complex valued functions u are square integrable on G. However, we prefer to use a more elegant, though more

abstract, way, considering the algebra $L^2(G)$ of square integrable complex functions with the convolution defined by the integral

$$(u \circ v)(g) = \int_G \mathrm{d}g'\, u(g')v(g'^{-1}g) \tag{6}$$

as a multiplication law [9, 11]. The $L^2(G)$ algebra is a Banach algebra with involution denoted by # and defined by the expression

$$u^*(g) = u^*(g^{-1}) \tag{7}$$

where * is the usual complex conjugation. It is worthwhile also to notice that $L^2(G)$ is the Hilbert space itself with the scalar product

$$(u\,|\,v)_2 = \int_G \mathrm{d}g\, u^*(g)v(g). \tag{8}$$

To construct now a collective space generated by the density operator ρ one needs to define a metastate on the algebra $L^2(G)$. Making use of the functional (2) by theorems IV.3.1–3.3 of [12] (see the appendix) one can write the metastate on $L^2(G)$ as the following integral

$$\langle \rho;\, u\rangle = \int_G \mathrm{d}g\, u(g)\langle \rho;\, T(g)\rangle \qquad \text{where } u \in L^2(G). \tag{9}$$

We used here the same clear notation for the functional on $\mathscr{A}(G)$ and the metastate on $L^2(G)$. In definition (9) it is assumed that $\langle \rho;\, T(g)\rangle$ is a square integrable function, i.e. it belongs to $L^2(G)$. Because the functional (2) is positively defined on $\mathscr{A}(G)$ the metastate (9) is also a positive functional on $L^2(G)$ i.e. $\langle \rho;\, u^* \circ u\rangle \geqslant 0$ for all $u \in L^2(G)$. The functional (9) could be used as a new, physical scalar product in $L^2(G)$ but it can happen that a non-zero vector could have the zero norm. To remove these pathological cases we use the standard GNS procedure. For this purpose we define the left-ideal in the algebra $L^2(G)$ that contains all the pathological elements

$$\mathscr{R}_\rho = \{u \in L^2(G) : \langle \rho;\, \alpha^* \circ u\rangle = 0 \text{ for all } \alpha \in L^2(G)\}. \tag{10}$$

For simplicity we refer to this ideal as a null-ideal for the density matrix ρ. Now the next step leads to the pre-Hilbert space $\mathscr{K}$ obtained as quotient algebra $L^2(G)/\mathscr{R}_\rho$, that after the standard procedure to complete it becomes the Hilbert space of states generated by the density operator ρ and the group of motions G. The scalar product in $\mathscr{K}$ is now defined by the metastate

$$(u\,|\,v)_{\mathscr{K}} = \langle \rho;\, u^* \circ v\rangle. \tag{11}$$

On the left-hand side of the definition (11), in principle one needs to write the classes of equivalent elements that are elements of the space $\mathscr{K}$. However, by tradition in quantum mechanics we write some of their representatives instead. The scalar product (11) can be rewritten in the form of double integral over the group manifold

$$(u\,|\,v)_{\mathscr{K}} = \int_G \mathrm{d}g' \int_G \mathrm{d}g\, u^*(g')\langle \rho;\, T(g'^{-1}g)\rangle v(g). \tag{11a}$$

This formula shows that the scalar product generated by the density operator is non-local, where the non-local kernel function is the generalized overlap function (GOF), that is a measure of coupling between 'deformations' g and g'. In order to

show that ρ generates the collective space we will find a link to the standard GCM approach. Let us consider the case of a pure state $\rho = |-\rangle\langle -|$, i.e. $\langle \rho;\ T(g)\rangle = \langle -|T(g)|-\rangle$, where $|-\rangle$ is a state vector belonging to the many-body Hilbert space $\mathcal{H}$. The proof that the element u belongs to the null ideal $\mathcal{R}_\rho$ if and only if the norm of the vector (1) with the generating function $T(g)|-\rangle$ in the many-body space is equal to zero, i.e. if

$$\left\| \int_G \mathrm{d}g\, u(g) T(g)|-\rangle \right\|_{\mathcal{H}} = 0 \tag{12}$$

is given in the appendix. This means that the space

$$\mathcal{H}_\rho = \left\{ \int_G \mathrm{d}g\, u(g) T(g)|-\rangle \colon u \in \mathcal{R}_\rho \right\} \tag{13}$$

corresponds exactly to the null space of the GCM method. It implies that the completed quotient space $\mathcal{H}_{\mathrm{GCM}} = \mathcal{H}/\mathcal{H}_\rho$, i.e. the collective space obtained from the GCM approach is isomorphic to the space $\mathcal{H} = L^2(G)/\mathcal{R}_\rho$. This isomorphism is given by

$$\tau \colon \mathcal{H} \ni u \to |{}^T u\rangle = \int_G \mathrm{d}g\, u(g) T(g)|-\rangle. \tag{14}$$

One can directly show that it conserves the scalar product; it has the same value in both spaces $\mathcal{H}$ and in the many-body one:

$$(u\,|\,v)_{\mathcal{H}} = \langle {}^T u\,|\,{}^T v\rangle \tag{15}$$

i.e. the transformation τ is unitary. This proves the equivalence of both spaces: the standard GCM space and the space obtained by the procedure given above with the metastate generated by the density operator $\rho = |-\rangle\langle -|$. In this way we see that instead of the standard GCM procedure one can use algebraic techniques that are more powerful than the older approach. In general, we define the metastate making use of the formulae (2) and (9) and we create the appropriate collective space $\mathcal{H}$.

In many applications it is important to know how the group G acts onto the collective states $\mathcal{H}$. We define the action by the left shift operators as follows:

$$\mathcal{L}^L(g')u(g) = u(g'^{-1}g) \qquad \text{where } u \in \mathcal{H}. \tag{16}$$

A direct calculation (see appendix) shows that the representation (16) is unitary and for the case of a pure state generating the collective space the unitary operator τ, equation (14), is a unitary isomorphism, i.e.

$$\tau \mathcal{L}^L(g) = T(g)\tau \tag{17}$$

and the representation $\mathcal{L}^L$ and T are unitarily, physically equivalent.

The formulation of AGCM allows for direct generalization of the Griffin–Hill–Wheeler (GHW) equations in the case of the collective space generated by ρ. It is also possible to derive the collective Hamiltonian within the Gaussian overlap approximation applying directly the formulae obtained in [3] with new GOF instead of a traditional overlap function. The GHW equation can be expressed as

$$\int_G \mathrm{d}g' \langle \rho;\ T(g)^+ H T(g')\rangle u(g') = E \int_G \mathrm{d}g' \langle \rho;\ T(g)^+ T(g')\rangle u(g') \tag{18}$$

with $u \in L^2(G)$, and the collective GOA Hamiltonian has the form

$$H_{\mathrm{coll}} = \mathcal{T} + \mathcal{V} + \mathcal{F} \tag{19}$$

where the collective kinetic energy operator is the second-order differential operator

$$\mathcal{T} = -\tfrac{1}{2}|\gamma|^{-1/2}\frac{\partial}{\partial q_k}\gamma^{1/2}(\mathcal{M}^{-1})_{kl}\frac{\partial}{\partial q_l} \tag{20}$$

in which γ_{kl} is the appropriate GOA metric tensor calculated with GOF and $(\mathcal{M}^{-1})_{kl}$ denotes the collective mass obtained by the formula given in [3] with substitution of the reduced energy kernel by our generalized energy kernel defined as follows:

$$h(g, g') = \frac{\langle \rho;\, T(g)^{+} H T(g')\rangle}{\langle \rho;\, T(g)^{+} T(g')\rangle} \tag{21}$$

where $g = g(q_1, \ldots, q_r)$, i.e. the parameters q_k parametrize the group elements and they stand for the collective variables. The collective potential $\mathcal{V}$ consists of the average energy of the system calculated with the density operator ρ corrected by the so-called zero-point energy. The asymmetry operator $\mathcal{F}$ in most cases disappears but it can be derived analogously.

3. The collective space and the collective energy

Now we are ready to construct an explicit realization of the collective space and calculate the collective energy. For the sake of simplicity we consider here a special but often-met case. Let us denote by $|\mu\, A\, a\rangle$ the eigenbasis of H; where μ denotes an invariant with respect to G set of quantum numbers, 'A' labels the irreducible representations of G and 'a' denotes a set of remaining quantum numbers required for unique specification of the basis for irreducible representation 'A' of G. In addition we assume that the density operator is also diagonal in the eigenbasis of H, e.g. ρ is a function of the Hamiltonian. According to our assumptions the following relations are fulfilled:

$$\rho|\mu\, A\, a\rangle = \rho(\mu A a)|\mu A a\rangle \tag{22}$$

$$H|\mu\, A\, a\rangle = E(\mu A a)|\mu A a\rangle. \tag{23}$$

We further define the so-called overlap operator known also in standard GCM, as follows:

$$(\mathcal{N}u)(g) = \int_G \mathrm{d}g' \langle \rho;\, T(g^{-1}g')\rangle u(g'). \tag{24}$$

The operator $\mathcal{N}$ is the continuous, Hermitian and positive operator in $L^2(G)$. In addition, it commutes with the representation $\mathcal{L}^L$ and because of the fact that the group G is compact it is of Schmidt–Hilbert type (appendix). Using the overlap operator, the scalar product in $\mathcal{H}$ one can write in the following way

$$(u|v)_{\mathcal{H}} = \langle \rho;\, u^{*} \circ v\rangle = \int_G \mathrm{d}g\, u^{*}(g)(\mathcal{N}v)(g). \tag{25}$$

Because of continuity of the overlap operator $\mathcal{N}$ the functional (25) as a functional of u, with fixed v function, is also continuous. By theorem IV.3.2 of [12] (see the appendix), to find the null ideal $\mathcal{R}_\rho$ it is enough to solve the homogeneous overlap equation

$$\mathcal{N}u = 0. \tag{26}$$

In our case the equation can be easily solved in the same way as in the paper [5]. One can calculate even more. Because the operator $\mathcal{N}$ is of Schmidt-Hilbert type operator it has only discrete series of eigenvalues and its eigenstates can be used as a basis in the collective space $\mathcal{K}$. One can also note that the action of the group G onto the states $|\mu Aa\rangle$ is, by their definition, given by

$$T(g)|\mu Aa\rangle = \sum_{a'} D^{A}_{a'a}(g)|\mu Aa'\rangle \tag{27}$$

where $D^{A}_{b'b}$ are the matrix elements of the irreducible representation A of the group G. The eigenvalues problem of the overlap operator can now be solved making use of the expansion of the searched eigenfunctions in the matrix elements $D^{A}_{b'b}(g)$ [5]. After some algebra the solutions of the eigenproblem of the overlap operator

$$\begin{aligned}(\mathcal{N}u^{A}_{aa'})(g) &\equiv \int_{G} \mathrm{d}g'\, \mathrm{Tr}(\rho T(g^{-1}g'))u_{aa'}(g') \\ &= \Lambda(Aa')u_{aa'}(g)\end{aligned} \tag{28}$$

in our case determined by equation (22), can be found in the form:

$$u^{A}_{aa'}(g) = (\dim_G[A])^{1/2} D^{A*}_{aa'}(g)$$

$$\Lambda(Aa') = \frac{\Sigma_\mu \rho(\mu Aa')}{\dim_G[A]}$$

where $\dim_G[A]$ denotes the dimension of the irreducible representation A and Tr is the trace calculated within the space created by the vectors $|\mu Aa\rangle$. The collective space is now spanned by all eigenvectors (more precisely by their classes that are elements of the quotient space $L^2(G)/\mathcal{R}_\rho$) $u^{A}_{aa'}(g)$ for that $\Lambda(Aa') \neq 0$. One can show directly that the vectors (for non-zero Λ)

$$e^{A}_{aa'}(g) = \Lambda(Aa')^{-1/2} u^{A}_{aa'}(g) \tag{29}$$

furnish the orthonormalized basis in $\mathcal{K}$. The states (29) correspond to the so-called natural states in the standard GCM approach. The collective Hamiltonian of our system can be now obtained by the projection of the Hamiltonian (23) onto the collective space $\mathcal{K}$. For this purpose it is sufficient to calculate the matrix elements of the Hamiltonian (23) within the states (29). The result of these calculations is given below:

$$\begin{aligned}H_{(Aaa')(Aa_1a_1')} &= \frac{1}{\sqrt{\Lambda(Aa')\Lambda(Aa_1')}} \langle \rho;\, e^{*}_{aa'} \circ He_{a_1a_1'}\rangle \\ &= \delta_{aa_1}\delta_{a'a_1'} \frac{\Sigma_\mu \rho(\mu Aa')E(\mu Aa)}{\Sigma_\mu \rho(\mu Aa')}.\end{aligned} \tag{30}$$

The matrix elements between the vectors belonging to different irreducible representations vanish, i.e. for $A \neq A'$. It means that the collective Hamiltonian obtained by the projection of the Hamiltonian (23) is diagonal in the basis (29) and the matrix elements (30) are equal to the collective energies. The collective energies (30) are labelled by three sets of quantum numbers: A, that denotes the irreducible representation of the group G and two sets of additional quantum numbers a and a', where a is required to distinguish states within a given irreducible representation A. The set of extra quantum numbers a' describes some internal motions of the system in respect to the group of motion G. The well known example of such a type of quantum number is

the number K representing a projection of the angular momentum vector onto an internal axis in the asymmetric top [13]. This dependence on the internal collective quantum numbers is a very interesting feature of the formalism and requires further investigation.

4. An illustration: [SU(6) ⊃ SU(5) ⊃ SO(5) ⊃ SO(3)]—interacting boson system

In this section we illustrate our considerations by a simple example. This example allows us to show another feature of the formalism developed in previous sections.

Let us consider the model of interacting bosons system consisting of a finite number of bosons N. The bosons occupy two levels with angular momenta $l=0$ (s-bosons) and $l=2$ (d-bosons), as in the popular nuclear collective model of interacting bosons (IBM) [14]. Let us assume that the metastate of the boson system is determined by a canonical density operator ρ. The dynamical symmetry of the system is the six-dimensional unitary group SU(6). For simplicity the Hamiltonian we choose to be diagonal within the following group chain

$$\mathrm{SU}(6) \supset \mathrm{SU}(5) \supset \mathrm{SO}(5) \supset \mathrm{SO}(3). \tag{31}$$

The quadrupole bosons are characterized here by their number n that ranges from 0 to N and their seniority v that changes from n, with step -2, to 0 or 1. The quantum number x distinguishes the equivalent representations for a given seniority and has the physical meaning of the maximum number of boson triplets coupled to the total angular momentum zero [15]. It ranges from 0 to the integer part of $v/3$. To complete the description of states there are two additional well known numbers: the total angular momentum quantum number L and its projection M. The selection rules for these are as follows:

$$\begin{aligned} &v-3x \leqslant L \leqslant 2(v-3x) \\ &L \neq 2(v-3x)-1. \end{aligned} \tag{32}$$

Thus, the quantum state is denoted by the ket $|NnvxLM\rangle$ and the full group of motion is SU(6) and the numbers N, n, v, L denote the irreducible representations in the group chain (31). Using the notation of [14] the eigenvalues of the interacting d-boson Hamiltonian can be written in the following simple expression:

$$E = E_{\mathrm{SU}(6)} + E_{\mathrm{SU}(5)} + E_{\mathrm{SO}(5)} + E_{\mathrm{SO}(3)} \tag{33}$$

where E_G denote the energies that can be expressed by the Casimir operators of the corresponding groups

$$E_{\mathrm{SO}(3)} = \gamma L(L+1)$$

$$E_{\mathrm{SO}(5)} = -\beta v(v+3)$$

$$E_{\mathrm{SU}(5)} = \varepsilon n + \frac{\alpha}{2} n(n-1) + \beta n(n+3) - 6\gamma n$$

$$E_{\mathrm{SU}(6)} = E_{\mathrm{SU}(6)}(N).$$

Now, using the formulae derived in the previous paragraph, we can calculate the energy spectra generated by every subgroup of the group SU(6) contained in the subgroups chain (31). We define the metastate for this system in the form of the canonical density matrix

$$\rho \equiv \frac{1}{\mathscr{Z}} \exp(-\theta H) \tag{34}$$

where H is the Hamiltonian corresponding to the eigenenergies (33). The parameter $T = 1/\theta$ we will call here 'a boson temperature', though the concept of temperature for this case seems to be problematic and requires further discussion. The $E_{SU(6)}$ term denotes an explicit dependence on the total number of bosons. We write down this term in the formulae for completeness, however in the energies calculations this term, to be consistent with (31), is neglected. Now we are able to write down the expressions for the motions generated by the groups SO(3), SO(5) and SU(5). Physically, this means that we impose some constraints on the quantum motion of d- and s-bosons. The constraints are strongest for the group SO(3), where finally not more than three degrees of freedom survive, i.e. the motion is constrained to rotations only. The SO(5) motion is connected with larger collective manifold: these SO(5) rotations can change the angular momentum but they keep the constant boson seniority number. The group of motion SU(5) is the dynamical symmetry group for the five-dimensional harmonic oscillator and describes the quadrupole vibrations with a fixed number of the quadrupole bosons. The detailed analysis of the collective manifolds corresponding to these groups of motion is an interesting problem. However it is beyond the scope of the present paper.

Therefore, the rotational 'temperature'-dependent energy can be written in a rather compact form:

$$\mathscr{E}_{SO(3)}(L, M_1, M_2) = E_{SO(3)}(L) + \frac{\sum_{Nnvx} e^{-\theta(E_{SU(6)}(N)+E_{SU(5)}(n)+E_{SO(5)}(v))} \times (E_{SU(6)}(N)+E_{SU(5)}(n)+E_{SO(5)}(v))}{\sum_{Nnvx} e^{-\theta(E_{SU(6)}(N)+E_{SU(5)}(n)+E_{SO(5)}(v))}}. \tag{35}$$

Here and below we write the summation over N only for formal reasons. In fact, by assumption N is fixed, and the summation over N disappears. The SO(5) rotations produce a richer spectrum that includes a possible coupling of pure rotational states to the additional degrees of freedom offered by the SO(5) motion. The energies corresponding to the SO(5) motion are as follows:

$$\mathscr{E}_{SO(5)}(v, x_1 L_1 M_1, x_2 L_2 M_2) = E_{SO(5)}(v) + E_{SO(3)}(L_1) + \frac{\sum_{Nn} e^{-\theta(E_{SU(6)}(N)+E_{SU(5)}(n))}(E_{SU(6)}(N)+E_{SU(5)}(n))}{\sum_{Nnxv} e^{-\theta(E_{SU(6)}(N)+E_{SU(5)}(n))}}. \tag{36}$$

The SU(5) allows for a full quadrupole motion. The appropriate energies can be written

$$\mathscr{E}_{SU(5)}(n, v_1 x_1 L_1 M_1, v_2 x_2 L_2 M_2) = E_{SU(5)}(n) + E_{SO(5)}(v_1) + E_{SO(3)}(L_1) + \frac{\sum_N e^{-\theta E_{SU(6)}(N)} E_{SU(6)}(N)}{\sum_N e^{-\theta E_{SU(6)}(N)}}. \tag{37}$$

As was mentioned above, the summation over N has in fact only one term and the last term reduces to $E_{SU(6)}(N)$ and the SU(5) energies are not dependent on the 'boson temperature'.

In all three formulae one can notice the appearance of the additional quantum numbers: for SO(3) group it is M_2, for SO(5) group we find x_2, L_2 and M_2 and for SU(5), in addition v_2. However, because of the form of the boson Hamiltonian the energies are independent of these additional quantum numbers. In another case one would expect an appearance of some bands dependent on them.

The eigenenergies in the limit $T \to 0$ are of great interest. For $T = 0$ the density operator ρ becomes the projection operator describing the ground state of N bosons, namely

$$\rho(T=0) = |N00000\rangle\langle N00000|.$$

The states of the form $|N00000\rangle$ are invariant under all subgroups in the chain (31), i.e. in respect of SU(5), SO(5) and SO(3). These subgroups are not able to excite the ground state (as in the case of the spherical quantum object with zero total angular momentum it is not possible to rotate it by the rotational operator to get higher angular momenta) and by the GCM procedure one cannot obtain any other states from it. Here we obtained the non-trivial spectra for all subgroups (figure 1) as the limit $T \to 0$.

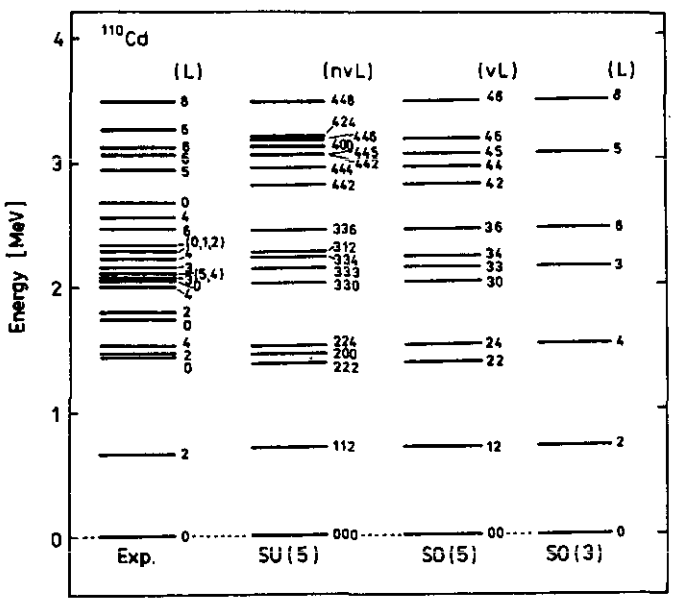

Figure 1. In the figure a scheme of the AGCM classification of the energy levels of the considered boson system is shown. The parameters for the Hamiltonian are taken from [14] as for ^{110}Cd nucleus calculated within so-called 'vibrational limit'.

In figure 1 one can notice the origin of the levels: some of them are generated from the ground state by the rotational group SO(3), some by SO(5) and some 'require' SU(5) to be excited. For instance, the SO(3)-levels with $L = 0, 2, 4, 6, 8$ have exactly the same energy as the SO(5)-levels with $L = 2v$. About these and other levels that survive after reduction of the collective degrees of freedom from SO(5) to SO(3) one

can say that they are quantum rotational states. After reduction from SU(5) to SO(5) motion also a set of states survives. Within this set there are some states that disappear after the next reduction to SO(3), e.g. the state $v=2$, $x=0$ and $L=2$. These states can be interpreted as the pure SO(5) excitations. The same analysis can be carried out for the SU(5) and so on. This procedure permits a division of the whole spectrum into subspectra generated by the appropriate groups of motions. This way one can introduce a new classification of the excitations.

In figure 2 we have plotted the behaviour of the eigenlevel energies as a function of 'boson temperature'. As was mentioned earlier the SU(5)-spectrum does not change with 'temperature' while using the Hamiltonian (33) and reproduces the full SU(6) spectrum. However, the energy spectra generated by SO(5) and SO(3) groups are 'temperature'-dependent. In figure 2 one can notice weaker dependence of the SO(5)-spectrum on the 'boson temperature' than that of the SO(3). It is a typical behaviour that can be explained by the fact that every SO(3)-state is a combination of all SU(6) states belonging to the irreducible representations $[N]$ with a given angular momentum, but the SO(5)-states are only the appropriate combinations of the states with fixed v, x and L. In the figure one can see that in our case the minimum of the ground state coincides with $T=0$. On the other hand, the parameter T can be treated as a new free parameter of the formalism allowing fitting of the metastate to the experimental data together with the Hamiltonian parameters. In this case the minimum of the ground state energy could be reached for $T>0$. These problems require further investigation for realistic models.

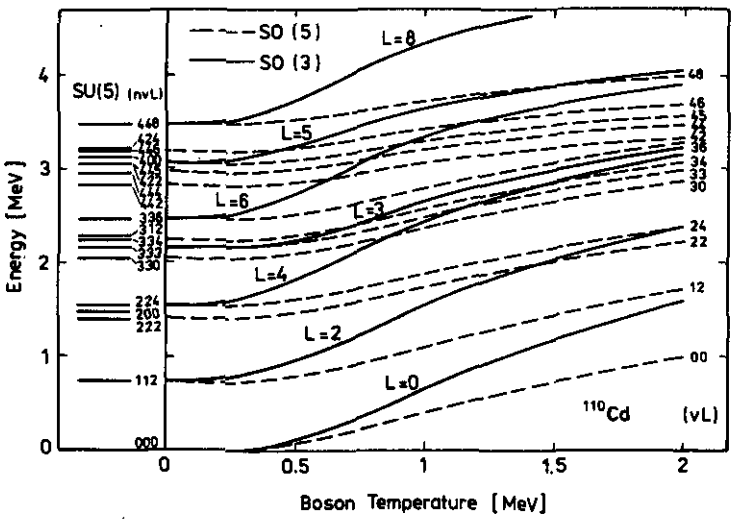

Figure 2. A dependence of the SO(3) and SO(5) spectra on the 'boson temperature' for the same set of parameters as in figure 1.

5. Conclusions

The AGCM method allows for construction of the spaces of states generated by a density matrix and a given group of motions. The structure of the states space is dependent on the shape of the metastate which, in turn, can be dependent on some external

parameters. This property of the formalism should, in principle allow for description of the phenomena for which the state space of a system is changing during the process.

This algebraical approach gives a tool for classification of the energy spectra with respect to subgroups of the group of motions, giving also information about the states internal structure—in other words, by reduction of the degrees of freedom (constraints) one can conclude which kind of motion is responsible for the given energy level. In addition, in some cases one can obtain a double set of quantum numbers generated by the group of motion G—the second set is responsible for an internal structure of the physical system and allows for the appearance of extra bands, like rotational K-bands in the asymmetric top.

To calculate by means of AGCM using the well known techniques of the GCM method in numerical codes for Griffin–Hill–Wheeler equations or in GOA approximation it is enough to change the overlap function and the reduced energy kernel.

In this paper we have mentioned a number of open problems that indicate certain directions for further investigation using the algebraic generator coordinate method, which seems to be a promising approach to many-body problems.

Appendix

In the appendix we give more detailed information of a rather more formal nature. The first problem is connected with equations (12) and (13). We have proved here the following:

Lemma. Let $\mathcal{R}_\rho$ denote the null-ideal for the metastate generated by a pure state $\rho = |-\rangle\langle -|$. The algebra element u belongs to $\mathcal{R}_\rho$ if and only if the corresponding many-body state, i.e. $\int_G \mathrm{d}g\, u(g)T(g)|-\rangle$ is the null vector in the many-body (GCM) state space.

Proof. If $u \in \mathcal{R}_\rho$ then $\mathcal{N}u = 0$, i.e. $\langle -|T(g)^+ \int_G \mathrm{d}g'\, u(g')T(g')|-\rangle = 0$ for every g. Multiplying both sides of this equation by $u^*(g)$ and after integration with respect to g we obtain $\|\int_G \mathrm{d}g\, u(g)T(g)|-\rangle\|_{\mathcal{H}} = 0$. The symbol $\mathcal{H}$ denotes here the many-body Hilbert space. Conversely, by multiplying $\int_G \mathrm{d}g\, u(g)T(g)|-\rangle = 0$ by the appropriate conjugated element one can obtain the equation $\langle \rho; v^* \circ u\rangle = 0$ for every $v \in L^2(G)$ that implies $u \in \mathcal{R}_\rho$.

The group action in the collective space $\mathcal{H}$ is given by equation (16). This representation is unitary. This statement can be proven by direct calculation of the scalar product

$$(\mathcal{L}^L u|\mathcal{L}^L v)_{\mathcal{H}} = \langle \rho; (\mathcal{L}^L u)^* \circ (\mathcal{L}^L v)\rangle.$$

The above written form can be expressed as a double invariant integral as in equation (11a), and by invariance of the Haar measure in respect of the left shift operator $\mathcal{L}^L$ it is equal to $(u|v)_{\mathcal{H}}$.

The property (17) comes from direct calculations and the lemma.

The properties of the overlap operator (24) can be determined on the basis of the following facts:

(a) The operator $\mathcal{N}$ is continuous in $L^2(G)$ (equivalently bounded) because the group G is compact and the integral kernel $\langle \rho; T(g^{-1}g')\rangle$ is bounded (4).

(b) $\mathcal{N}$ is the Hermitian operator because the integral kernel is also Hermitian.

(c) From the relation $(u|\mathcal{N}u)_{L^2(G)} = \langle \rho; u^* \circ u\rangle \geq 0$ it can be seen that the overlap operator is positive.

(*d*) The definition (24) and properties *a* and *b* determine (see [16]) that the operator $\mathcal{N}$ is of Schmidt-Hilbert type.

The theorems 3.1–3.3 from chapter IV of [12] are essential for proofs of some statements in the paper. For readers' convenience we have translated these theorems from [12].

Theorem 3.1. Assume the measure μ is totally σ-finite, y denotes a measurable function and the integral $\int_G d\mu(g)x(g)y(g)$ exists and is finite for every $x \in L^p(G)$ then $y \in L^q(G)$, where $1/p+1/q=1$.

Theorem 3.2. Given a continuous linear functional $\langle y; \rangle$ defined on $L^p(G)$, there exists one and only one element $y \in L^q(G)$ that

$$\langle y; u\rangle = \int_G d\mu(g)x(g)y(g) \qquad (*)$$

for $x \in L^p(G)$. The norm of this functional is equal to $\|y\|_q$. Conversely, every functional of the form (*) is linear and continuous in $L^p(G)$.

Theorem 3.3. The operation A which associates every $y \in L^q(G)$ with the functional $\langle y; \rangle$ on the space $L^p(G)$, $1<p<\infty$, by the formula

$$\langle y; x\rangle = \int_G d\mu(g)x(g)y(g)$$

is the isometric map from $L^q(G)$ to $L^p(G)^*$ (the asterisk denotes here an adjoint space).

References

[1] Hill D L and Wheeler J A 1953 *Phys. Rev.* **89** 112
Griffin J J and Wheeler J A 1957 *Phys. Rev.* **108** 311
[2] Ring P and Schuck P 1980 *The Nuclear Many-Body Problem* (Berlin: Springer)
[3] Góźdź A 1985 *Phys. Lett.* **152B** 281–3
Góźdź A, Pomorski K, Brack M and Werner E 1985 *Nucl. Phys.* A **442** 26–49, 50–67
Góźdź A and Pomorski K 1986 *Nucl. Phys.* A **451** 1–10
Łojewski Z and Góźdź A 1988 *Phys. Lett.* **213B** 107
[4] de Toledo Piza A F R, de Passos E J V, Galetti D, Nemes M C and Watanabe M M 1977 *Phys. Rev.* C **15** 1477
de Toledo Piza A F R and de Passos E J V 1978 *Nuovo Cimento* B **45** 1
[5] Góźdź A 1989 *Acta Phys. Pol.* B **20** 235–42
[6] Emch G G 1972 *Algebraic Methods in Statistical Mechanics and Quantum Field Theory* (New York: Wiley-Interscience)
[7] Bratteli O and Robinson D W 1979 *Operator Algebras and Quantum Statistical Mechanics 1* (New York: Springer)
[8] Sudbery A 1986 *Quantum Mechanics and the Particles of Nature* (Cambridge: Cambridge University Press)
[9] Kirillov A A 1978 *Eliemienty tieorii priedstavlienij* (Moscow: Nauka)
[10] Żelazko W 1968 *Algebry Banacha* (Warsaw: PWN)
[11] Hartman S 1969 *Wstęp do analizy harmonicznej* (Warsaw: PWN)
[12] Alexiewicz A 1969 *Analiza funkcjonalna* (Warsaw: PWN)
[13] Eisenberg J M and Greiner W 1970 *Nuclear Theory* vol I (Amsterdam: North-Holland)
[14] Arima A and Iachello F 1976 *Ann. Phys.* **99** 253
[15] Szpikowski S and Góźdź A 1980 *Nucl. Phys.* A **340** 76
Góźdź A 1986 *Acta Phys. Pol.* B **18** 258
[16] Mlak W 1972 *Wstęp do teorii przestrzeni Hilberta* (Warsaw: PWN)