AN APPLICATION OF GROUP THEORY TO THE GENERATOR COORDINATE METHOD*

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(Received October 19, 1988)

In the paper the generator coordinate method is reformulated to show its symmetry conservation property. The equations for the eigenvalues and eigenvectors of an overlap operator for the case of compact groups are derived. A rotational motion of an axially symmetric nuclear system is considered.

PACS numbers: 21.60.–n, 21.60.Ev

1. Introduction

The generator coordinate method (GCM) is a well known standard method allowing to find the energy spectra of many physical systems by solving the integral Hill-Wheeler equation [1, 2]. This method, however, should be rather treated as a very powerful projection method which simultaneously excludes the irrelevant variables from the wave function of a system under consideration [3]. To show this property more clearly one needs to reformulate the GCM approach as follows [4]. Let us denote a generator function by the ket

$$|q\rangle = |q^1, q^2, \ldots, q^s\rangle \tag{1}$$

and define the hermitian, non-negative overlap operator acting in the many-body state space $\mathscr{K}$:

$$\mathscr{N} = \int_\Omega dq |q\rangle \langle q|, \tag{2}$$

where $dq = \varrho(q) dq^1 dq^2 \ldots dq^s$ stands for a volume element in the integral. For simplicity in notation we assume that the operator $\mathscr{N}$ has only discrete spectrum (a continuous case can be treated in the same way), i.e.

$$\mathscr{N}|n\rangle = \Lambda(n)\,|n\rangle. \tag{3}$$

* Supported in part by the Polish Ministry of Education, Project CPBP 01.09.

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It is interesting that for the operator $\mathcal{N}$ one can define a "brother" operator $\mathcal{N}_{\text{coll}}$ acting in the space $\mathcal{H}_{\text{coll}} \subset L^2(\Omega)$ of the functions $f(q)$:

$$(\mathcal{N}_{\text{coll}} f)(q) := \int_{\Omega} dq' \langle q|q'\rangle f(q'). \tag{4}$$

The subscript coll means 'collective' because in most applications in nuclear physics the space obtained by this procedure is a space of the collective motions.

Let us denote by $w_n(q)$ and λ_n the eigenfunctions and the eigenvalues of $\mathcal{N}_{\text{coll}}$, respectively. From the spectral theorem one can expand the overlap function as follows

$$\langle q|q'\rangle = \sum_m \lambda_m w_m(q) w_m^*(q'). \tag{5}$$

This decomposition allows to prove that the, so called, "natural states" in GCM defined by the equation

$$|n\rangle = \{\lambda_n\}^{-1/2} \int_{\Omega} dq w_n(q) |q\rangle \tag{6}$$

are the eigenfunctions of the overlap operator (2), i.e.

$$\Lambda(n) = \lambda_n, \tag{7}$$

and the transformation

$$U: w_n \to |n\rangle \tag{8}$$

defined by the Eq. (6) is one-to-one and unitary. In other words, the spaces $\mathcal{H}_{\text{ccll}}$ spanned by the eigenfunctions $\{w_n(q)\}$ belonging to the nonzero eigenvalues and $\mathcal{H}_P = \Sigma |n\rangle \langle n| \mathcal{H} = P\mathcal{H}$ spanned by the natural states (6) are unitarily, i.e. physically, equivalent. This important property is a base of application of GCM in description of a nuclear collective motion. It is much easier to perform calculations and to interpret results in the space $\mathcal{H}_{\text{coll}}$ than in the equivalent many-body subspace $\mathcal{H}_P$.

2. Lie groups and symmetries in GCM

In many practical cases the generator function is of the form

$$|\alpha, q\rangle = T(\alpha) |q\rangle, \tag{9}$$

where $T(\alpha)$ stands for an unitary operator representation of a locally compact Lie group G in the state space $\mathcal{H}$, $\alpha \in G$. The letter q represents a set of additional generator coordinates. For this case the overlap operator can be written as a double integral

$$\mathcal{N} = \int_G d\mu(\alpha) \int_{\Omega} dq T(\alpha) |q\rangle \langle q| T^{\dagger}(\alpha), \tag{10}$$

where $\int d\mu(\alpha)$ denotes an invariant integral over the group G [5]. Using properties of the Haar measure one can prove by computation that the operator $\mathcal{N}$ is invariant under group transformations, namely

$$T(\alpha) \mathcal{N} T^{\dagger}(\alpha) = \mathcal{N}. \tag{11}$$

This symmetry property of the operator $\mathcal{N}$ causes that its eigenvalues are dependent only on the sets of quantum numbers I labelling the unitary irreducible representations of G and the quantum numbers χ connected with the collective variables q and they are independent of the sets M of numbers distinguishing the basis vectors within the same irreducible representation I

$$\mathcal{N}|IM;\chi\rangle = \Lambda(I\chi)\,|IM;\chi\rangle. \tag{12}$$

The operator P which projects onto the many-body collective subspace $\mathcal{H}_P = P\mathcal{H}$, unitarily equivalent to the collective space $\mathcal{H}_{\text{coll}} \subset L^2(G \cup \Omega)$, can be written in the form

$$P = \sum_{IM\chi} |IM;\chi\rangle\langle IM;\chi|, \quad \Lambda(I\chi) \neq 0. \tag{13}$$

The invariance property (11) implies invariance of the projection operator P. The same symmetry properties can be proved for the transformation U. However, it acts between two different spaces and this feature must be expressed in a slightly different form, namely

$$T(\alpha)UT^{\dagger}_{\text{coll}}(\alpha) = U, \tag{14}$$

where $T_{\text{coll}}(\alpha) = U^{\dagger}T(\alpha)U$ is a unitary operator representation of the group G in the collective space $\mathcal{H}_{\text{coll}}$.

In the following we assume that the group G is a symmetry group of a hamiltonian H. The collective many-body hamiltonian H_P can be obtained by the projection of H onto the space $\mathcal{H}_P$

$$H_P = PHP. \tag{15}$$

From earlier discussion it is obvious that H_P is invariant under action of the symmetry group G

$$T(\alpha)H_PT^{\dagger}(\alpha) = PT(\alpha)HT(\alpha)P = H_P. \tag{16}$$

Finally, because of (14), also the collective hamiltonian

$$\mathcal{H} = U^{\dagger}H_PU \tag{17}$$

has the same symmetry group as the projected hamiltonian (15) and the original hamiltonian H.

Consider now the generator function of type (9) but with fixed variables q

$$|\alpha\rangle = T(\alpha)\,|-\rangle,\ \alpha \in G. \tag{18}$$

The invariance property of the Haar measure allows to write the operator $\mathcal{N}_{\text{coll}}$ in the following form

$$(\mathcal{N}_{\text{coll}}f)(\alpha) = \int_G d\mu(x)\,\langle -|T(x)\,|-\rangle\,(\alpha x), \tag{19}$$

where $f \in \mathcal{H}_{\text{coll}} \subset L^2(G)$. For the compact group (below we consider only the compact groups because for the noncompact case one needs to use more sophisticated methods

of the group theory) by Peter-Weyl theorem [5] the eigenfunctions w_{IM} of $\mathcal{N}_{\text{coll}}$ can be expanded in the matrix elements of the unitary irreducible representations of G:

$$w_{IM}(\alpha) = \sum_K c^I_{MK} \sqrt{\dim (I)}\, [D^I_{MK}(\alpha)]^*, \tag{20}$$

where $\dim (I)$ denotes the dimension of the irreducible representation I. After straightforward calculations, from (19) and (20) one obtains the set of equations for the eigenvalues $\Lambda(I, \chi)$ and coefficients c^I_{MK}:

$$\sum_K c^I_{MK} \left\{ \frac{\langle - | P^I_{MK} | - \rangle}{\dim (I)} - \Lambda(I)\delta_{KK'} \right\} = 0 \tag{21}$$

with the normalization condition $\sum_K |c^I_{MK}|^2 = 1$, where

$$P^I_{MK} := \dim (I) \int_G d\mu(\alpha) D^{I*}_{MK}(\alpha) T(\alpha)$$

are the projection operators [5]. Using the states (6) the eigenvectors of the overlap operator $\mathcal{N}$ can be expressed as

$$|IM\rangle = \{\Lambda(I)\}^{-1/2} \sum_K \frac{c^I_{MK}}{\sqrt{\dim (I)}} P^I_{MK} | - \rangle. \tag{22}$$

The collection of states (22), for non-zero eigenvalues $\Lambda(I)$, furnishes a basis of the many-body collective subspace $\mathcal{H}_P$. The corresponding basis in $\mathcal{H}_{\text{coll}}$ is given by Eq. (20).

3. The nuclear rotations

Now we consider the rotational motion of the axially symmetric nuclei with fixed deformation. The generator function is assumed in the form (18) with an axially symmetric internal state $| - \rangle$

$$|\Omega\rangle = R(\Omega) | - \rangle, \tag{23}$$

where $R(\Omega)$ is the usual rotation operator and Ω denotes the set of Euler angles. This choice of the generator function allows to search for all possible rotational states contained in the ket $| - \rangle$. Using the formulae from (19) to (22) we obtain:

$$w_{JM}(\Omega) = \sqrt{2I+1}\, D^{J*}_{M0}(\Omega), \tag{24a}$$

$$\Lambda(J) = \int_{SO(3)} d\Omega \langle - | R(\Omega) | - \rangle D^{J*}_{00}(\Omega) \tag{24b}$$

and

$$|JM\rangle = \{\Lambda(J)\}^{-1/2} \int_{SO(3)} d\Omega w_{JM}(\Omega) R(\Omega) | - \rangle, \tag{24c}$$

where

$$\int_{SO(3)} d\Omega = \frac{1}{8\pi^2} \int_0^{2\pi} d\Omega_1 \int_0^{\pi} d\Omega_2 \sin \Omega_2 \int_0^{2\pi} d\Omega_3. \tag{24d}$$

Note, that the expressions (24) are the same when we replace the group SO(3) by SU(2) (one needs only to change one limit of integration from 2π to 4π and to double the volume of a group manifold from $8\pi^2$ to $16\pi^2$). The operator which projects onto the rotational space $\mathscr{K}_P$ can be constructed from the states (24c)

$$P = \sum_{JM} |JM\rangle \langle JM|, \quad J \in Q, \tag{25}$$

where Q denotes the set of the angular momentum quantum numbers J which are allowed by the structure of the internal function $|-\rangle$. In the following we assume that the nuclear hamiltonian H is rotationally invariant, then

$$\langle J'M'|PHP|JM\rangle = \delta_{JJ'}\delta_{MM'}E_J \tag{26}$$

with the rotational energy

$$E_J = \frac{1}{\Lambda(J)} \int_{SO(3)} d\Omega \langle -|HR(\Omega)|-\rangle D^{J*}_{00}(\Omega). \tag{27}$$

The projected, rotational hamiltonian can thus be written as

$$PHP = \sum_{J \in Q} (E_J - E_{g.s.}) P^J + E_{g.s.} P, \tag{28}$$

where

$$P^J = \sum_M |JM\rangle \langle JM|, \quad J \in Q. \tag{29}$$

The operator P^J is chosen in the Löwdin form [6]:

$$P^J = \prod_{\substack{I \in Q \\ I \neq J}} \frac{\hat{J}^2 - I(I+1)}{J(J+1) - I(I+1)}. \tag{30}$$

Here, $\hat{J}^2$ means square of the total angular momentum operator restricted to the collective subspace $\mathscr{K}_P$. Because of invariance property of the operators $\mathscr{N}$, $\mathscr{N}_{coll}$, P and U one can easily transform P^J to the space $\mathscr{K}_{coll}$. It is enough to replace the operator $\hat{J}^2$ by its realization $\hat{J}^2(\Omega) = U^\dagger \hat{J}^2 U$ on the group manifold of the group SO(3), i.e. by its standard representation through the Euler angles. This transformation leads to the explicit form of the collective rotational hamiltonian in the space $\mathscr{K}_{coll}$:

$$\mathscr{H} = \sum_{J \in Q} (E_J - E_{g.s.}) \prod_{\substack{I \in Q \\ I \neq J}} \frac{\hat{J}^2(\Omega) - I(I+1)}{J(J+1) - I(I+1)} + E_{g.s.} \tag{31}$$

$$= E_{g.s.} + \tfrac{1}{2} \mathscr{I}^{-1} \hat{J}^2(\Omega) + \ldots, \tag{31}$$

where the moment of inertia

$$\mathscr{I} = \left\{ 2 \sum_{J \in Q} (E_J - E_{g.s.}) \left| \sum_{\substack{I' \in Q \\ I' \neq J}} \frac{\prod_{\substack{I \in Q \\ I \neq J, I'}} [-I(I+1)]}{\prod_{I \neq J} [J(J+1) - I(I+1)]} \right| \right\}^{-1}. \tag{32}$$

is explicitly dependent on the energetical structure of all levels in a rotational band. This formula can be used directly to calculate a moment of inertia for a given band from the experimental data instead of the phenomenological expression dependent only on the first excited state in the band, i.e. $\mathscr{I}_{2^+} = 3/(E_{2^+} - E_{g.s.})$. For a ground state band satisfying the standard energetical relations for a rotor both moments of inertia $\mathscr{I}$ and $\mathscr{I}_{2^+}$ coincide. In other cases one obtains some differences.

As an example we consider a ground state rotations for the nucleus ^{8}Be. The generator function $|\Omega; \alpha\rangle$ is chosen in the form (23) with internal function *parametrically* dependent on a deformation α generated by a scaling operator

$$S = \sum_i \left(z_i \frac{\partial}{\partial z_i} - \tfrac{1}{8} \sum_j z_i \frac{\partial}{\partial z_j} \right). \tag{33}$$

The generator function is now given by

$$|\Omega; \alpha\rangle = R(\Omega) \alpha^{-7/2} \exp\left[-(\ln \alpha) S\right] |\Phi_0\rangle, \tag{34}$$

where

$$\Phi_0 = (8!)^{-1/2} \det |(\phi_0 \phi_1)^4| \tag{35}$$

is the Slater determinant consisting of the usual three-dimensional harmonic oscillator eigenstates in the Cartesian basis. The superscript 4 in (35) indicates that the four spin-isospin combinations occur with the same orbital states. Making use of the overlap functions calculated by Arickx, Broeckhove and Deumens [7] one can immediately get the rotational energies of the nucleus ^{8}Be shown in Fig. 1. In the calculations a semi-realistic two-body interaction of BB1 force by Brink and Boeker [8] has been used. To have non-spurious results the center of mass motion has been taken into account. In Fig. 1 the ground state energy $E_{g.s.}$ is plotted as a function of the deformation parameter α. The minimal ground state energy has been achieved for $\alpha_{eq} = 1.6$ and $E_{g.s.}(1.6) = -50.33$ MeV. The experimental value of the binding energy is equal 56.7 MeV, however, BB1 forces do not contain the Coulomb interaction and, in fact, one has to compare $E_{g.s.}(1.6)$ with ≈ 60 MeV of the binding energy increased by the Coulomb energy. For the equilibrium deformation, we also plotted the rotational band obtained from the calculations and compared with experimental data. The agreement between both spectra is good. In Fig. 2 the shape of energy spectrum as a function of the deformation parameter α is shown. In the figure all bound states obtained from calculations are plotted. One can observe strong compression of a spectrum for the spherical case, $\alpha = 1$. In this case only two excited levels are bounded. When the deformation grows two additional levels 6^+ and 8^+ descend to the bound states region.

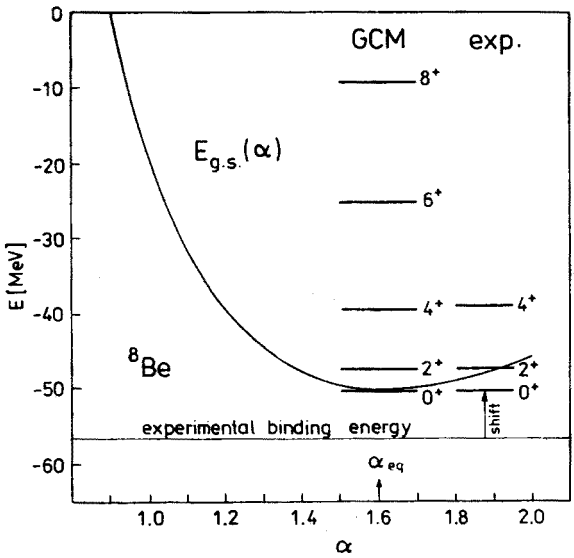

Fig. 1. The ground state energy of ^{8}Be as a function of deformation α. The experimental and the calculated rotational spectra are compared. The experimental 0^+ level is shifted to the calculated one

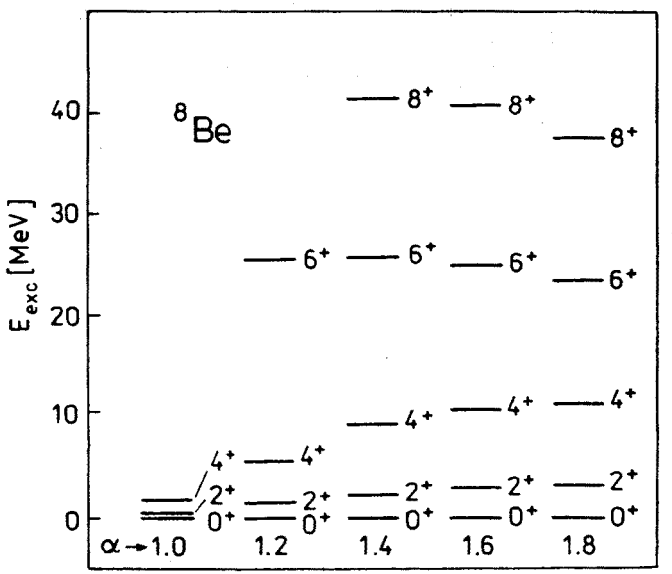

Fig. 2. The calculated spectrum as a function of deformation for ^{8}Be nucleus

4. Summary and remarks

To obtain more complete spectrum of ^{8}Be one has to consider the additional degrees of freedom, e.g. one can treat the parameter α as a second generator coordinate. However, because the scaling operator (32) generates a non-compact group the procedure given above must be modified. This will be a subject of a subsequent paper. In this paper a general

proof of the fact that the generator coordinate method conserves the symmetries of the original hamiltonian is sketched. A method of construction of a many-body collective subspace for a collective motion generated by a compact Lie group is presented. On the example of nuclear rotational motion a more detailed procedure to obtain a corresponding collective hamiltonian in the space $\mathscr{K}_{\text{coll}}$ is shown. This procedure can be used for an arbitrary compact Lie group. The general method allows for different approximations. One possible approximation which conserves the symmetry properties of the general formalism is the extended Gaussian overlap approximation [9, 10] succesfully applied to the description of nuclear collective motion [11–12]. Another approximation scheme based on the projection of a total hamiltonian onto a space spanned by the polynomials of a Lie group generators is in preparation. It seems that this method could allow to use more realistic then the single-particle hamiltonians without time consuming numerical calculations. This program, however, requires further investigations.

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