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The Geometric Content of the Interacting Boson Model for Molecular Spectra.
A Testground for the Nuclear IBM.

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Abstract

The recently proposed algebraic model for collective spectra of diatomic molecules is analysed in terms of conventional geometrical degrees of freedom. We present a mapping of the algebraic Hamiltonian onto an exactly solvable geometrical Hamiltonian with the Morse potential. This mapping explains the success of the algebraic model in reproducing the low lying part of molecular spectra. At the same time the mapping shows that the expression for the dipole transition operator in terms of boson operators differs from the simplest IBM expression and in general must include many-body boson terms. The study also provides an insight into the problem of possible interpretations of the bosons in the nuclear IBM.

1. Introduction

The interpretation of the algebraic Interacting Boson Model¹⁾ (IBM) in terms of an underlying dynamical or geometrical picture is an issue which has recently attracted much attention²⁻⁷⁾. The link which was suggested between the IBM and the Bohr-Mottelson⁸⁾ picture is an important step towards our better understanding of the IBM in the framework of concepts familiar from the Bohr-Mottelson approach.

Recently, Iachello⁹⁾ proposed an Interacting Boson Model description of the rotation-vibration spectra of diatomic molecules. The results bear an impressive resemblance to the observed spectra, which is of the same quality as in the applications of the IBM in the nuclear case. The main difference between the nuclear and molecular problems is that for the latter one has an established dynamical theory. Thus the molecular IBM offers a testground where our geometrical and dynamical interpretations of the IBM can be studied. This note reports the results of such an investigation.

We start in Section 2.1 by a brief review of the molecular IBM. In Section 2.2 we use the methods of Ref. (7) and discuss the transformation to the conventional geometrical variables. Section 2.3 deals with the $O(4)$ limit of the molecular IBM. In this limit it is possible to find a mapping of the algebraic Hamiltonian onto a solvable Hamiltonian with the Morse potential. This mapping is used in Section 2.4 in the discussion of the dipole transition operator. Section 2.5 presents a brief analyses of the $U(3)$

symmetry limit of the molecular IBM. This limit is analogous to the vibrational U(5) limit of the nuclear IBM. In the last section we summarize some general conclusions which pertain not only to the molecular theory but also to the nuclear problem.

2.1 - The Algebraic Model

In the application of the IBM to the molecular problems Iachello⁹⁾ proposed the use of the U(4) dynamical algebra, which is realized in terms of four pairs of boson creation and annihilation operators, σ , σ^+ and π_μ , π_μ^+ ($\mu = -1, 0, 1$). The σ -bosons are assumed to transform under rotations as scalars, while π_μ transform as spherical components of a vector.

The molecular model Hamiltonian H is constructed in such a way that the total number of bosons

$$N = \sigma^+ \sigma + \sum_{\mu=-1}^1 \pi_\mu^+ \pi_\mu \quad (2.1)$$

is conserved.

Under the limitation of at most quartic boson-boson interactions (i.e. bosons interact pairwise) one considers two possible dynamical symmetries built upon the following chains of subgroups of U(4)

$$a) U(4) \supset O(4) \supset O(3) \quad (2.2a)$$

$$b) U(4) \supset U(3) \supset O(3) \quad (2.2b)$$

When the Hamiltonian is constructed as a linear combination of the Casimir operators of the corresponding subgroups (2.2a) or (2.2b) the energy spectrum can be found in an analytic form by group-theoretical methods⁹⁾. In analogy with the nuclear IBM we refer to the chains (2.2a) and (2.2b) as the $O(4)$ -symmetry and the $U(3)$ -symmetry, respectively.

The spectrum of the $O(4)$ symmetry is especially relevant to the molecular problem. The Hamiltonian is written⁹⁾ as

$$H = A P_4 + B C_3 \quad (2.3)$$

where A and B are adjustable constants and P_4 is the boson pairing operator

$$P_4 = S_+ S_- \quad (2.4a)$$

with

$$S_+ = \frac{1}{2} \left[\sum_{\mu=-1}^1 (-1)^{\mu} \pi_{\mu}^+ \pi_{\mu}^+ - \sigma^+ \sigma^+ \right] \quad (2.4b)$$

$$S_- = (S_+)^+$$

In Eq.(2.3) C_3 is the Casimir operator of $O(3)$, i.e. the angular momentum J^2

$$C_3 \equiv J^2 = \text{const} \left\{ [\pi^+ \times \tilde{\pi}]^{(0)} \cdot [\pi^+ \times \tilde{\pi}]^{(0)} \right\} \quad (2.5a)$$

with

$$\tilde{\pi}_{\mu} = (-1)^{J+\mu} \pi_{-\mu} \quad (2.5b)$$

The Hamiltonian (2.3) is very similar to the O(6) symmetry in the nuclear IBM and can be diagonalized⁹⁾ in exactly the same way with the result

$$E(0(4)) = \frac{1}{4} A (N-S)(N+S+2) + BJ (J+1) \quad (2.6a)$$

where N is the boson number and S = N, N-2, ... 1 or 0 for N odd or even.

The angular momentum J takes the values,

$$J = S, S-1 \dots 0. \quad (2.6b)$$

The comparison with molecular spectra is facilitated by the introduction of the vibrational quantum number $v = \frac{1}{2} (N - S)$ so that $v_{\max} = N/2$ or $(N-1)/2$ is the total number of vibrational states. In terms of v the expression (2.6a) becomes

$$E(0(4)) = A(N+1) v - Av^2 + B J(J+1) \quad (2.7)$$

Simple diatomic molecules (e.g. H_2) display rotational-vibrational spectra which resemble closely the spectrum (2.7). It has a finite number of bound vibrational states, quadratic anharmonicities in the dependence on the vibrational quantum number for low lying states and a moment of inertia which is to a good approximation constant, independent of v . The last feature is of course the reflection of a negligible rotational-vibrational coupling for the low lying states.

The structure of the dipole transition operator in terms of the boson operators σ and π_μ is not determined by the choice of the boson Hamiltonian. Rather, it is constructed independently and represents an additional assumption of the model. The most simple candidate can be chosen as a linear combination of the three possible hermitian one-body boson operators

$$d_\mu^{(1)} = \pi_\mu^+ G + \widetilde{\pi}_\mu G^+ \quad (2.8a)$$

$$d_\mu^{(2)} = i (\pi_\mu^+ G - \widetilde{\pi}_\mu G^+) \quad (2.8b)$$

$$d_\mu^{(3)} = (\pi_\mu^+ \times \widetilde{\pi}_\mu)_\mu^{(4)} \quad (2.8c)$$

where $d_\mu^{(3)}$ is proportional to the operator of the angular momentum. There are no apriory reasons to limit oneself to one-body operators. We discuss this particular choice because of its relevance to the nuclear IBM where as a rule the electromagnetic transition operators are taken to be of a one-boson character. We focus our attention on the operator

$d_{\mu}^{(1)}$, Eq. (2.8a). This operator is a generator of the O(4) algebra and therefore has vanishing matrix elements between rotational bands of (2.7) with different vibrational quantum numbers. This feature has analogy with the quadrupole operator in the O(6) limit and in the rotational SU(3) limit of the nuclear IBM¹⁾.

The reduced matrix elements of the operator (2.8a) within a given rotational band are

$$\begin{aligned} & \langle [N], v, J \| d^{(1)} \| [N], v, J+1 \rangle = \\ & = \text{const} (J+1)^{1/2} [(N-2v+1)^2 - (J+1)^2]^{1/2} \end{aligned} \quad (2.9)$$

They include a typical IBM cutoff factor which decreases when the quantum numbers J or v increase.

2.2 Geometrical Variables

In the present section we shall transform the algebraic Hamiltonian and express it in terms of geometrical variables. In doing so, we follow closely the procedure of ref.(7). It is most convenient to perform the transformation to the geometrical variables by first passing to the classical limit of the IBM. This is obtained by simply replacing the boson operators $\sigma, \sigma^+, \pi_{\mu}, \pi_{\mu}^+$ in the Hamiltonian by classical, commuting variables, which we denote respectively as $\alpha_0, \alpha_0^*, \alpha_{\mu}$ and α_{μ}^* . (we set $\hbar=1$ throughout this work). The formal justification for this intuitively obvious replacement was reviewed in Chapter 2.1 of Ref.(7).

The boson number operator (2.1) has the classical limit

$$N(\alpha) = \alpha_G^* \alpha_G + \sum_{\mu=-1}^1 \alpha_\mu^* \alpha_\mu \quad (2.10a)$$

The commutation of N with the IBM Hamiltonian implies that the corresponding classical quantity $N(\alpha)$ is conserved as can be also verified directly by evaluating $dN(\alpha)/dt$ and using the Hamilton equations of motion for the canonical variables α_G, α_μ and $i\alpha_G^*, i\alpha_\mu^*$.

The cyclic variable Q canonically conjugate to $N(\alpha)$ is

$$Q = i \ln \sqrt{\frac{\alpha_G}{\alpha_G^*}} \quad (2.10b)$$

The Hamiltonian obviously does not depend on Q . We will use N and Q as a new pair of canonical variables.

In the nuclear case the next step in the procedure of Ref. (7) was to form combinations of α 's which could be regarded as the nuclear quadrupole deformations. In the molecular context the geometrical variables describing the collective vibrations and rotations are obviously related to the three components of the vector distance between the atoms in a diatomic molecule. We therefore seek for such combinations q_μ of the α 's which satisfy the usual conditions

$$q_\mu = (-1)^{1+\mu} q_{-\mu}^* \quad (2.11)$$

for the spherical components of a vector. An obvious choice is

$$q_{\mu} = \frac{1}{\sqrt{2}} \left(\alpha_{\mu}^* \sqrt{\frac{\alpha_{\sigma}}{\alpha_{\sigma}^*}} + (-1)^{+\mu} \alpha_{-\mu} \sqrt{\frac{\alpha_{\sigma}}{\alpha_{\sigma}^*}} \right) \quad (2.12a)$$

with the canonically conjugate momenta

$$p_{\mu} = -\frac{i}{\sqrt{2}} \left(\alpha_{\mu} \sqrt{\frac{\alpha_{\sigma}^*}{\alpha_{\sigma}}} - (-1)^{+\mu} \alpha_{-\mu}^* \sqrt{\frac{\alpha_{\sigma}^*}{\alpha_{\sigma}}} \right) \quad (2.12b)$$

Inverting the transformation (2.10, 2.12)

$$\begin{aligned} \alpha_{\mu} &= \frac{1}{\sqrt{2}} (q_{\mu}^* + i p_{\mu}) e^{-iQ} \\ \alpha_{\sigma} &= e^{-iQ} \sqrt{N - \frac{1}{2} \sum_{\mu} (p_{\mu} p_{\mu}^* + q_{\mu} q_{\mu}^*)} \end{aligned} \quad (2.13)$$

one can easily verify that $i\alpha_{\sigma}^* \dot{\alpha}_{\sigma} + \sum_{\mu} i\alpha_{\mu}^* \dot{\alpha}_{\mu}$ differs from $N\dot{Q} + \sum_{\mu} p_{\mu} \dot{q}_{\mu}$ by a total time derivative, as is required for a canonical transformation.

Having defined the spherical components q_{μ} we can further transform them to cartesian coordinates,

$$q_{\pm 1} = \mp \frac{i}{\sqrt{2}} (x \pm iy), \quad q_0 = iz, \quad (2.14a)$$

with the canonical momenta

$$p_{\pm 1} = \pm \frac{i}{\sqrt{2}} (p_x \mp i p_y), \quad p_0 = -i p_z. \quad (2.14b)$$

It will be more convenient to work in spherical coordinates for which the corresponding transformation is

$$q_{\pm 1} = \mp \frac{i}{\sqrt{2}} r \sin \vartheta e^{i\varphi} \quad (2.15a)$$

$$q_0 = i r \cos \vartheta, \quad ,$$

and

$$p_{\pm 1} = \pm \frac{i}{\sqrt{2}} \left(p_r \sin \vartheta + \frac{p_\vartheta}{r} \cos \vartheta \mp \frac{i p_\varphi}{r \sin \vartheta} \right) e^{\mp i\varphi} \quad (2.15b)$$

$$p_0 = -i \left(p_r \cos \vartheta - \frac{1}{r} p_\vartheta \sin \vartheta \right).$$

Here we use the obvious notation for r, θ and ϕ and the corresponding momenta p_r, p_θ and p_ϕ .

In the following sections we will analyze the molecular IBM by passing first to the classical variables $\alpha_\sigma, \alpha_\sigma^*, \alpha_\mu, \alpha_\mu^*$ and then transforming them to the geometrical variables defined by the relations (2.13-15). Working with classical variables enables us to perform these canonical transformations in a straightforward way.

The presence of the square root in (2.13) imposes limitations on the range of variations of the geometrical variables introduced in (2.15).

Transforming the expression under the square root one obtains the following constraint

$$p_r^2 + r^2 + \frac{J^2}{r^2} \leq 2N \quad (2.16)$$

It is difficult to implement this constraint in a precise quantitative way. In practical applications however the boson number N is very large (~ 30) and in the forthcoming discussion we will disregard (2.16), allowing thereby for relative errors of the order N^{-1} .

2.3 - The $O(4)$ Symmetry

The algebraic Hamiltonian in this case is given by Eq. (2.3-5). Following the procedure of the previous section we replace the boson operators by the classical variables $\alpha_\sigma, \alpha_\mu$ and use the transformations (2.13) and (2.15). After some lengthy but straightforward algebra we obtain the following expression for the $O(4)$ Hamiltonian in the geometrical variables

$$H_c(O(4)) = \frac{A}{4} [r^2 p_r^2 + (r^2 - N)^2] + B J^2, \quad (2.17a)$$

where r and p_r are the radial coordinate and momentum and J^2 is expressed via the angular geometrical variables in the usual way.

$$J^2 = p_\vartheta^2 + \frac{p_\varphi^2}{\sin^2 \vartheta} \quad (2.17b)$$

It is perhaps not surprising that the radial part of (2.17a) formally coincides with that of the O(6) Hamiltonian for the nuclear IBM⁷⁾, with B and p_B replaced by r and p_r .

The equilibrium in the radial variables occurs at $p_r=0$ and $r=\sqrt{N}$. One can analyze Eq. (2.17a) by expanding around this point and using the fact that N is very large ($\sim 25 - 30$) in actual applications⁹⁾. A more straightforward procedure however can be followed which seems to be especially suited for the molecular case. We wish to transform the kinetic energy in (2.17a) to a quadratic dependence on the momentum with a constant mass coefficient. This is achieved by the point transformation

$$\rho = -2 \ln(r/\sqrt{N}), \quad p_\rho = -\frac{1}{2} r p_r, \quad (2.18)$$

where ρ and p_ρ are the new canonical variables.

The Hamiltonian (2.17a) becomes

$$H_\rho = A p_\rho^2 + \frac{AN^2}{4} (1 - e^{-\rho})^2 + B J^2 \quad (2.19)$$

with the desired form of the kinetic energy. At the same time the potential energy has become precisely the Morse potential¹⁰⁾ which is widely used as a valid approximation to the actual interatomic potential of diatomic molecules. In this approximation one writes the radial part of the 3-dimensional molecular Hamiltonian as

$$H_{\text{Morse}}(R) = \frac{p_R^2}{2m} + V_{\text{Morse}}(R) + \frac{J^2}{2m R^2} \quad (2.20a)$$

with

$$\begin{aligned}
 V_{\text{Morse}}(R) &= D(\exp[-2a(R-R_0)] - 2\exp[-a(R-R_0)]) = \\
 &= -D + D(\exp[-a(R-R_0)] - 1)^2 \quad (2.20b)
 \end{aligned}$$

We denote here by R the internuclear distance, D is the dissociation energy and R_0 is the equilibrium distance.

The relation between the Morse Hamiltonian (2.20a) and the Hamiltonian (2.19) can be established in the following way. One first neglects the rotational-vibrational coupling by setting $R=R_0$ in the centrifugal term of (2.20a) and obtaining thereby a constant moment of inertia. The next step, discussed in Ref.(11) is to regard the first two terms in (2.20a) as a one dimensional Hamiltonian ignoring the polar nature of the coordinate R and extending its range to $-\infty \leq R \leq \infty$. A similar approximation must be invoked also in the Hamiltonian (2.19). According to (2.18) and (2.16) the maximum range of ρ is $-\infty \leq \rho \leq \infty$. For large N and energies not too high above the minimum of the potential one can replace the lower bound on ρ by $-\infty$.

Under these approximations and correlating the parameters such that

$$\begin{aligned}
 a(R - R_0) &\rightarrow \rho \\
 \frac{a^2}{2m} &\rightarrow A \\
 D &\rightarrow AN^2/4 \\
 1/2m R_0^2 &\rightarrow B
 \end{aligned} \quad (2.21)$$

one finds that the Hamiltonian (2.20) is identical to (2.19) up to an additive constant $(-D)$. Accounting for this constant and for the relations (2.21) one also finds that the known exact spectrum of the one dimensional Morse oscillator¹⁰⁾

$$E_v = -\frac{a^2}{2m} (v - v_{max})^2, \quad v_{max} = \frac{\sqrt{2mD}}{a} - \frac{1}{2} \quad (2.22)$$

coincides with the v -dependent part of the algebraically derived expression (2.7) for the $O(4)$ symmetry spectrum (a small difference of the order N^{-1} reflects our way of analyses through the classical limits).

The foregoing discussion shows clearly what is the dynamical basis of the algebraic $O(4)$ symmetry in the molecular IBM. It consists of

- a) choosing the Morse potential to describe the diatomic molecule,
- b) neglecting the rotational-vibrational coupling and
- c) treating the radial equation as one dimensional. These approximations reduce the model to an exactly solvable problem. The resulting spectrum yields quite an accurate description for the low lying part of the molecular spectrum.

2.4 - The Dipole Transition Operator

As was already indicated in Section 2.1 the choice of the transition operators in algebraic models is not dictated by the Hamiltonian and must be made independently as a part of the formulation of the model. This choice can be made on physical grounds only if one specifies what are the dynamical degrees of freedom which are algebraically represented

in terms of boson operators. We will use the relation between the algebraic $O(4)$ model and the Morse Hamiltonian (2.20) found in the last section in order to discuss this problem.

For the molecular Hamiltonian (2.20) a very good approximation for the operator describing the dipole transitions between the low lying states is given by $\gamma \vec{R}$ where γ is a constant and \vec{R} is the vector distance between the nuclei. The radial part $R = |\vec{R}|$ of this operator determines the "intrinsic" dipole moments of the rotational bands and the interband transitions. The relations (2.21) and (2.18) show that in terms of the geometrical variables (2.15a) the operator R is

$$R = -\frac{2}{\alpha} \ln r + \left(r_0 + \frac{\ln N}{\alpha} \right) . \quad (2.23)$$

Expressing this in terms of the boson operators of the algebraic model results in an infinite series of one-body, two-body, etc. terms. We are not able to exhibit this transformations explicitly. Instead we will examine the matrix elements of the operator R and compare them with the one body boson operator (2.8a), which is of the type used in the nuclear IBM.

The exact matrix elements of R between the states of the Morse oscillator were calculated in Ref.(12) and are given by fairly complicated expressions. Their trend can be studied on the basis of simple considerations, based on a harmonic approximation to the Morse potential (2.20b). Calculating the second derivative at the equilibrium point one finds that the frequency of small vibrations around R_0 is

$$\omega = \sqrt{\frac{2Da^2}{m}} \quad (2.24)$$

In this approximation

$$\langle v+1 | R | v \rangle = \sqrt{\frac{v+1}{2m\omega}} \quad , \quad (2.25)$$

and the "intrinsic" dipole moment

$$\langle v | R | v \rangle = R_0 \quad (2.26)$$

is independent of v . The ratio of the intensities of the interband to the intraband transitions is therefore

$$\left[\frac{\langle v+1 | R | v \rangle}{\langle v | R | v \rangle} \right]^2 = \frac{v+1}{2mR_0^2\omega} = \frac{B(v+1)}{AN} \quad (2.27)$$

In the last equality we used the correspondence (2.21) between the Morse Hamiltonian and the parameters of the $O(4)$ Hamiltonian. For $v=0$ the ratio (2.27), although small, is of the same order of magnitude as the ratio of the rotational to the vibrational part in the energy spectrum (2.7) of the algebraic model. The neglected rotational-vibrational coupling terms are of higher order $\sim (B/AN)^2$. Since the operator $d^{(1)}$ of Eq. (2.8) is a generator of $O(4)$ its matrix elements for the interband transitions vanish identically. This is inconsistent with the orders of magnitude estimate given above.

In the harmonic approximation the intrinsic dipole moment (2.26) is independent of v . At the same time the $O(4)$ spectrum contains anharmonic vibrational term $\sim v^2$ which is of the relative order N^{-1} . We are therefore led to investigate the effect of unharmonicities on the matrix elements of the dipole operator R . The cubic term in the expansion of the Morse potential around R is $-D a^3 (R - R_0)^3$. Denoting by $|\delta v\rangle$ the correction to the harmonic wave-function $|v\rangle$ due to this term we find the following relative correction to the intrinsic dipole moment

$$\begin{aligned} \frac{2 \langle \delta v | R | v \rangle}{\langle v | R | v \rangle} &= \frac{18 D a^3}{m^2 R_0 \omega^3} (2v + 1) = \\ &= \frac{18}{N} \sqrt{\frac{B}{A}} (2v + 1) \end{aligned} \quad (2.28)$$

where we used first order perturbation theory and the relations (2.21) for the parameters. Eq. (2.28) shows an intuitively expected increase of the dipole moment with the value of v due to the anharmonic effects of the Morse potential. At the same time the expression (2.9) for the matrix elements of $d^{(1)}$ shows quite an opposite dependence on the vibrational quantum number v .

The dependence on the angular momentum J of the matrix elements of the dipole operator R is given by its angular part. It causes the $J \rightarrow J \pm 1$ transitions to have intensities proportional to $(J+1)$. This again differs from the intensities of similar transitions with the operator $d^{(1)}$, Eq. (2.9), where the cutoff factor decreases with the increase of J .

2.5 - The U(3) Symmetry

The algebraic Hamiltonian based upon the second chain (2.2b) of subgroups of U(4) generates a spectrum which does not have a counterpart in collective molecular spectra. It is however of interest because of its analogy to the vibrational U(5) limit in the nuclear IBM.

The simplest U(3) invariant Hamiltonian is of course the harmonic expression

$$H_0 = \varepsilon \sum_{\mu=-1}^1 \pi_{\mu}^+ \pi_{\mu} \quad (2.29)$$

In terms of the geometrical variables (2.15) this is

$$H_0 = \frac{\varepsilon}{2} \left(p_r^2 + \frac{J^2}{r^2} + r^2 \right) \quad (2.30)$$

with the constraint (2.16). Apart from this constraint, (2.30) is as expected just the Hamiltonian of the 3-dimensional harmonic oscillator with the equilibrium position at $r=0$.

The quartic anharmonic terms which can be added to the algebraic Hamiltonian (2.29) in a way consistent with the U(3) symmetry are

$$\sum_{L=0,2} C_L \left[(\pi^+ \times \pi^+)^{(L)} \times (\tilde{\pi} \times \tilde{\pi})^{(L)} \right]^{(0)}, \quad (2.31)$$

where C_L are arbitrary coefficients. Transforming to the geometrical variables one obtains

$$a \left(p_r^2 + \frac{J^2}{r^2} + r^2 \right)^2 + b J^2 \quad (2.32)$$

where a and b are linear combinations of the coefficients C_L . Thus the anharmonicities introduced by the IBM look very peculiar when expressed in terms of the geometrical degrees of freedom. They consist of the square of the harmonic Hamiltonian (2.30) and the conserved term J^2 . Although the terms (2.32) can produce a strongly anharmonic spectrum of energies, at the same time the dynamics of the harmonic limit remains completely unchanged. This conclusion matches the discussion of the U(5) limit in the nuclear IBM given in Ref.(7). As in the nuclear case the form (2.32) follows directly from the IBM restriction on the boson number conservation by the boson interactions. The natural anharmonic term $\sim r^4$ added to (2.30) would correspond to boson nonconserving interactions $\sim (\pi^+)^4$, $(\pi^-)^4$, etc., in the algebraic Hamiltonian.

3. Conclusions

In the preceding sections we have shown that by a series of transformations and reasonable approximations, one can map the algebraic Hamiltonian onto a geometrical Hamiltonian expressed in terms of simple dynamical degrees of freedom. This mapping should provide a guide in the construction of the algebraic counterparts of dynamical observables such as the dipole operator in the molecular IBM or the quadrupole operator in the nuclear IBM.

It is essential to recognize in this respect that the construction of the Hamiltonian which reproduces a given experimental spectrum within an Interacting

Boson Model is completely disconnected from the expression of dynamical observables (e.g. transition moments) within such a model. In our discussion of the $O(4)$ limit of the molecular IBM we saw that following the guide lines provided by the mapping onto a geometrical Hamiltonian brings about a complicated expression for the dipole operator in terms of bosons. We have also shown that the choice of the dipole operator in a standard IBM fashion (i.e. quadratic in boson operators) fails to reproduce the correct dependence of transition matrix elements on the quantum numbers.

Our discussion of the $U(3)$ limit shows that the p-boson conserving interactions produce terms which look rather unphysical when transformed to the geometrical variables. This emphasizes the fact that the boson operators with non zero angular momentum (i.e. p-bosons in the present molecular case) are ordinary vibrational phonons rather than real conserved bosons.

The conservation of the total boson number is meaningful only in the situations where the s-bosons appear explicitly in the Hamiltonian. Then for a fixed boson number N the s-bosons do not represent an independent degree of freedom and can be expressed in terms of N and the variables represented by the p-bosons, e.g. Eq. (2.13). Thus, the role of the s-boson can be viewed as a compact way of writing complicated interactions between the p-bosons which do not conserve their number and are in accordance with their interpretation as ordinary phonons. The cutoff factor introduced by fixing the total number N of bosons has no physical significance and effects only the high energy part of the spectrum where the model is not applicable.

Finally it is important to stress that in both the $U(3)$ and the $O(4)$ limits the p-bosons are vibrational phonons around the point $r=0$ in the corresponding geometrical picture. The p-boson interactions simulated by

the s-bosons in the $O(4)$ case move the equilibrium position to a non zero value of r , i.e. create a "deformed" equilibrium. Vibrations around this new equilibrium are complicated combinations of the original spherical phonons (p-bosons). This fact is reflected, for instance, in the corresponding expression for the dipole transition operator.

Upon completion of this work we have received a preprint of Ref. (13) where techniques similar to ours were used in order to investigate the applications of the semi-classical mean-field methods to algebraic Hamiltonians.

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