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Rotation–vibrational spectra of diatomic molecules and nuclei with Davidson interactions

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Abstract. Complete rotation–vibrational spectra and electromagnetic transition rates are obtained for Hamiltonians of diatomic molecules and nuclei with Davidson interactions. Analytical results are derived by dynamical symmetry methods for diatomic molecules and a liquid-drop model of the nucleus. Numerical solutions are obtained for a many-particle nucleus with quadrupole Davidson interactions within the framework of the microscopic symplectic model.

1. Introduction

Many interaction potentials have been considered for the relative dynamics of two-body systems (cf the comparative study by Varshni [1]). The most useful potentials are ones for which the radial Schrödinger equation is solvable by factorization [2] and/or algebraic methods [3]. These include the harmonic oscillator, Coulomb, Morse and Pöschl–Teller potentials (for a review of one-body problems solvable by algebraic and factorization methods, for example, the articles by Cooper [4] and Dutt *et al* [5]). However, with the exception of the harmonic oscillator and Coulomb potentials, algebraic solutions for three-dimensional systems are generally available only for angular momentum zero states. Thus there is a need for algebraically solvable potentials that apply to all angular momentum states and which, as a consequence, are useful for studying rotational systems and the manner in which they are perturbed by rotation–vibration interactions.

The rotational states of a truly rigid rotor can be handled easily [6]. However, the expansion on a vibrational basis of a rigid rotor wavefunction (which involves delta functions in the relative coordinates) does not converge to a square integrable wavefunction. By the same token, the eigenfunctions of a soft vibrational rotor are very slowly convergent in a spherical vibrational basis. This emphasizes the need for a model which gives a good first approximation for the states of a rotation–vibrational system and provides a meaningful basis for more realistic approximations.

In section 3, we consider algebraic solutions of a diatomic molecule with a potential

$$V(r) = \chi \left(r^2 + \frac{\varepsilon}{r^2} \right). \quad (1)$$

This potential was introduced by Davidson [7]. As a molecular interaction, it is unrealistic at large r values and has no unbound states. However, it has the distinct advantage that its Schrödinger equation has a complete set of algebraic solutions. Moreover, it can be handled algebraically in any number of dimensions.

In section 4, we consider a many-body system with Davidson interactions and show that it has an $\mathfrak{su}(1, 1) \times \mathfrak{so}(3)$ spectrum generating algebra. This enables one to derive the relative energies of states within a common $\mathfrak{su}(1, 1) \times \mathfrak{so}(3)$ irrep. However, we have not been able to derive the energy differences of states belonging to different many-particle irreps.

The model we consider has much in common with the Calogero model [8] which can be regarded as a model for many particles in a one-dimensional space with Davidson interactions. Our hope was that the special characteristics of the Calogero model, which render it accessible to algebraic solution, might be extendable to three dimensions. This does not appear to be the case. However, the rotations and vibrations of a many-particle nucleus, do have algebraic solutions within the framework of the Bohr–Mottelson collective model [9].

The Bohr–Mottelson model is a liquid-drop model with five collective quadrupole coordinates $\{q_\nu; \nu = 0, \pm 1, \pm 2\}$ and five canonical momentum coordinates $\{\pi^\nu = -i\hbar\partial/\partial q_\nu\}$. With the Hamiltonian

$$H_0 = \frac{1}{2B}\pi \cdot \pi + \frac{1}{2}B\omega^2 q \cdot q \quad (2)$$

it gives a harmonic vibrational spectrum. But, with a quadrupole Davidson potential, the Hamiltonian

$$H_\varepsilon = \frac{1}{2B}\pi \cdot \pi + \frac{1}{2}B\omega^2 \left(q \cdot q + \frac{\varepsilon}{q \cdot q} \right) \quad (3)$$

yields a rotation–vibrational spectrum characteristic of the so-called gamma-soft, Willets–Jean [10] limit of the collective model. This was shown by Elliott *et al* [11], who derived energy levels and collective model wavefunctions for such a potential by analytic methods. Algebraic solutions for this Hamiltonian are derived in section 5 using an $\mathfrak{su}(1, 1) \times \mathfrak{so}(3)$ spectrum generating algebra (cf [12]).

With quadrupole moments $\{Q_\nu\}$ for the nucleus expressed in the form

$$Q_\nu = \sqrt{\frac{16\pi}{5}} \sum_{n=1}^A r_n^2 Y_{2\nu}(\theta_n, \varphi_n) \quad (4)$$

where $(r_n, \theta_n, \varphi_n)$ are spherical polar coordinates of a nucleon, the Davidson potential

$$V(Q) = \chi \left(Q \cdot Q + \frac{\varepsilon}{Q \cdot Q} \right) \quad (5)$$

becomes a microscopic potential. Furthermore, since the $\{Q_\nu\}$ moments, as well as the many-nucleon kinetic energy $\sum_n p_n^2/2m$ and the harmonic oscillator potential $\frac{1}{2}m\omega^2 \sum_n r_n^2$, are elements of an $\mathfrak{sp}(3, \mathbb{R})$ Lie algebra, it follows that a complete set of many-nucleon eigenstates can be found for the unified model Hamiltonian

$$H = \frac{1}{2m} \sum_n p_n^2 + \frac{1}{2}m\omega^2 \sum_n r_n^2 + V(Q) \quad (6)$$

with each state lying within an irrep of the $\mathfrak{sp}(3, \mathbb{R})$ Lie algebra [13]. This makes it possible to carry out microscopic calculations of nuclear states for the Davidson potential within the framework of the symplectic model [13–15]. The symplectic model is discussed and preliminary results for the Davidson potential are given in section 7.

2. The spherical harmonic oscillator

The energy-level spectrum and eigenfunctions of the spherical harmonic oscillator can be constructed in many ways. A construction that survives the addition of a Davidson potential to the Hamiltonian is one that uses an $\text{Sp}(3, \mathbb{R}) \supset \text{Sp}(1, \mathbb{R}) \times \text{SO}(3)$ dynamical subgroup chain. Thus, before proceeding, we outline the use of this subgroup for the spherical harmonic oscillator.

Infinitesimal generators of $\text{Sp}(1, \mathbb{R})$ are given by

$$\begin{aligned}\hat{Z}_1 &= p^2 = \sum_i p_i^2 & \hat{Z}_2 &= r^2 = \sum_i x_i^2 \\ \hat{Z}_3 &= \frac{1}{2}(\mathbf{r} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{r}) = \frac{1}{2} \sum_i (x_i p_i + p_i x_i)\end{aligned}\quad (7)$$

where $\{\hat{x}_j, \hat{p}_j\}$ satisfy the Heisenberg commutation relations

$$[\hat{x}_j, \hat{p}_k] = i\hbar \delta_{jk} \hat{I}. \quad (8)$$

These operators span an $\mathfrak{sp}(1, \mathbb{R}) \sim \mathfrak{su}(1, 1)$ Lie algebra with commutation relations

$$\begin{aligned}[\hat{Z}_1, \hat{Z}_2] &= -4i\hbar \hat{Z}_3 & [\hat{Z}_3, \hat{Z}_1] &= 2i\hbar \hat{Z}_1 \\ [\hat{Z}_3, \hat{Z}_2] &= -2i\hbar \hat{Z}_2.\end{aligned}\quad (9)$$

The components of the angular momentum

$$\hbar \mathbf{L} = \mathbf{r} \times \mathbf{p} \quad (10)$$

likewise span the $\mathfrak{so}(3)$ Lie algebra.

The $\mathfrak{sp}(1, \mathbb{R})$ commutation relations can be brought to standard $\mathfrak{su}(1, 1)$ form by defining

$$\begin{aligned}\hat{X}_1 &= \frac{1}{4\hbar} \left(a\hat{Z}_1 - \frac{1}{a}\hat{Z}_2 \right) \\ \hat{X}_2 &= \frac{1}{2\hbar} \hat{Z}_3 & \hat{X}_3 &= \frac{1}{4\hbar} \left(a\hat{Z}_1 + \frac{1}{a}\hat{Z}_2 \right).\end{aligned}\quad (11)$$

We then obtain the familiar expressions

$$\begin{aligned}[\hat{X}_1, \hat{X}_2] &= -i\hbar \hat{X}_3 & [\hat{X}_2, \hat{X}_3] &= i\hbar \hat{X}_1 \\ [\hat{X}_3, \hat{X}_1] &= i\hbar \hat{X}_2.\end{aligned}\quad (12)$$

Positive discrete series irreps for $\mathfrak{su}(1, 1)$ are characterized by a lowest weight λ with positive real values. Orthonormal bases for these irreps are given by states $\{|n\lambda\rangle; n = 0, 1, 2, \dots\}$ which satisfy the equations

$$\begin{aligned}\hat{X}_+|n\lambda\rangle &= \sqrt{(\lambda+n)(n+1)}|n+1, \lambda\rangle \\ \hat{X}_-|n+1, \lambda\rangle &= \sqrt{(\lambda+n)(n+1)}|n\lambda\rangle \\ \hat{X}_0|n\lambda\rangle &= \frac{1}{2}(\lambda+2n)|n\lambda\rangle\end{aligned}\quad (13)$$

where

$$\hat{X}_\pm = \hat{X}_1 \pm i\hat{X}_2 \quad \hat{X}_0 = \hat{X}_3. \quad (14)$$

The latter operators obey the commutation relations

$$[\hat{X}_-, \hat{X}_+] = 2\hat{X}_0 \quad [\hat{X}_0, \hat{X}_\pm] = \pm\hat{X}_\pm. \quad (15)$$

If we set $a = 1/m\omega$ in equation (11) we find that

$$\hat{X}_0 = \hat{X}_3 = \frac{1}{2\hbar\omega} \left[\frac{1}{2m} p^2 + \frac{1}{2} m\omega^2 r^2 \right]. \quad (16)$$

The states $\{|n\lambda\rangle\}$ are then eigenstates of the harmonic oscillator Hamiltonian

$$\hat{H} = 2\hbar\omega\hat{X}_0 \quad (17)$$

with energies

$$E_{n\lambda} = (2n + \lambda)\hbar\omega. \quad (18)$$

Basis states $\{|nlm\rangle; n = 0, 1, 2, \dots, m = -l, \dots, +l\}$ for an $\mathfrak{su}(1, 1) \times \mathfrak{so}(3)$ irrep are obtained by raising with the $\mathfrak{su}(1, 1)$ raising operators from $n = 0$ lowest weight states $\{|0lm\rangle\}$. The latter states are annihilated by the $\mathfrak{su}(1, 1)$ lowering operator $\hat{X}_- = \hat{X}_1 - i\hat{X}_2$ and have wavefunctions ψ_{0lm} given in spherical polar coordinates by

$$\psi_{0lm}(r, \theta, \varphi) = N_l e^{-r^2/2\alpha} r^l Y_{lm}(\theta, \varphi) \quad (19)$$

where $\alpha = m\omega/\hbar$ is the square of the harmonic oscillator unit of length. These wavefunctions are eigenfunctions of the weight operator with eigenvalues given by

$$\hat{X}_0\psi_{0lm} = \frac{1}{4}(2l + 3)\psi_{0lm}. \quad (20)$$

Thus, for the spherical harmonic oscillator, $\lambda = l + \frac{3}{2}$ and

$$E_{nl} = (2n + l + \frac{3}{2})\hbar\omega. \quad (21)$$

3. Spectra for diatomic molecules

We now consider the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 \left(r^2 + \frac{\varepsilon}{r^2} \right) \quad (22)$$

for a diatomic molecule, where m is the reduced mass of the two atoms. The notation is simplified if the coordinates are expressed in harmonic oscillator units of length, for which $\hbar/m\omega = 1$. The Hamiltonian then becomes

$$H = \frac{1}{2}\hbar\omega \left(-\nabla^2 + r^2 + \frac{\varepsilon}{r^2} \right). \quad (23)$$

To find eigenstates of H , we again use the $\mathfrak{sp}(1, \mathbb{R})$ algebra. However, instead of the basis operators defined by equation (7), we consider

$$\begin{aligned} \hat{Z}'_1 &= \hat{Z}_1 + \frac{\hbar^2\varepsilon}{\hat{Z}_2} = \hbar^2 \left(-\nabla^2 + \frac{\varepsilon}{r^2} \right) & \hat{Z}'_2 &= \hat{Z}_2 = r^2 \\ \hat{Z}'_3 &= \hat{Z}_3 = -\frac{1}{2}i\hbar(\mathbf{r} \cdot \nabla + \nabla \cdot \mathbf{r}). \end{aligned} \quad (24)$$

The remarkable fact is that this nonlinear transformation leaves the $\mathfrak{sp}(1, \mathbb{R})$ commutation relations (9) invariant. Thus, the spectrum is given, as for the spherical harmonic oscillator, by an expression of the form

$$E_{nl} = [2n + \lambda(l)]\hbar\omega. \quad (25)$$

However, the harmonic oscillator relationship $\lambda(l) = l + \frac{3}{2}$ no longer applies.

The new relationship between λ and l can be inferred from the value of the $\mathfrak{su}(1, 1)$ Casimir invariant

$$\hat{C}_2 = \hat{X}_3^2 - \hat{X}_1^2 - \hat{X}_2^2 = \hat{X}_0(\hat{X}_0 - 2) - \hat{X}_+ \hat{X}_- \quad (26)$$

which takes n -independent values given by

$$\hat{C}_2|n\lambda\rangle = \frac{1}{4}\lambda(\lambda - 2)|n\lambda\rangle. \tag{27}$$

Thus, for the spherical harmonic oscillator, for which $\varepsilon = 0$, the operator takes values

$$C_2(\varepsilon = 0) = (l + \frac{3}{2})(l - \frac{1}{2}). \tag{28}$$

When $\varepsilon \neq 0$, the carrier spaces of the $\mathfrak{su}(1, 1)$ irreps remain the same. However, the Casimir operator changes because the realization of the $\mathfrak{su}(1, 1)$ algebra changes. In terms of the $\mathfrak{sp}(1, \mathbb{R})$ operators, we have

$$\hat{C}_2(\varepsilon) = \frac{1}{4\hbar^2} \left[\frac{1}{2}(\hat{Z}'_1\hat{Z}'_2 + \hat{Z}'_2\hat{Z}'_1) - \hat{Z}'_3{}^2 \right] = \hat{C}_2(\varepsilon = 0) + \frac{1}{4}\varepsilon \tag{29}$$

where

$$\hat{C}_2(\varepsilon = 0) = \frac{1}{4\hbar^2} \left[\frac{1}{2}(\hat{Z}_1\hat{Z}_2 + \hat{Z}_2\hat{Z}_1) - \hat{Z}_3{}^2 \right]. \tag{30}$$

Thus, the appropriate relationship between λ and l is given by

$$\lambda(l)(\lambda(l) - 2) = (l + \frac{3}{2})(l - \frac{1}{2}) + \varepsilon \tag{31}$$

which implies that

$$\lambda(l) = 1 + \sqrt{(l + \frac{1}{2})^2 + \varepsilon}. \tag{32}$$

It follows that the energy level spectrum for the Hamiltonian (22) is given by

$$E_{nl} = \left[2n + 1 + \sqrt{(l + \frac{1}{2})^2 + \varepsilon} \right] \hbar\omega. \tag{33}$$

Eigenfunctions of the Hamiltonian can be generated as easily as for the spherical harmonic oscillator. If we write the wavefunction ψ_{nlm} for the state $|nlm\rangle$ in terms of spherical polar coordinates,

$$\psi_{nlm}(r, \theta, \varphi) = e^{-r^2/2} P_{nlm}(r, \theta, \varphi) \tag{34}$$

it follows, from the condition that the lowest weight states $\{|0lm\rangle\}$ are annihilated by the $\mathfrak{su}(1, 1)$ lowering operator \hat{X}_- , that P_{0lm} satisfies the equation

$$\left[-\nabla^2 + \frac{\varepsilon}{r^2} \right] P_{0lm}(r, \theta, \varphi) = 0. \tag{35}$$

One easily shows that

$$\nabla^2 r^a (x + iy)^l = [a(a + 1) + 2la] r^{a-2} (x + iy)^l. \tag{36}$$

Thus, we obtain the solution to equation (35) with

$$P_{0lm}(r, \theta, \varphi) = N_l r^{a+l} Y_{lm}(\theta, \varphi) \tag{37}$$

where a is a solution of the equation

$$a(a + 1) + 2la - \varepsilon = 0. \tag{38}$$

It follows that

$$\psi_{0lm}(r, \theta, \varphi) = N_l e^{-r^2/2} r^{b_l} Y_{lm}(\theta, \varphi) \tag{39}$$

where N_l is norm factor

$$N_l = \left[\frac{2}{\Gamma(b_l + 2)} \right]^{1/2} \quad \text{and} \quad b_l = \sqrt{[(l + \frac{1}{2})^2 + \varepsilon]} - \frac{1}{2}. \tag{40}$$

Note that we choose the solution for which $a > 0$ so that the wavefunction is well defined for small r and the norm factor is obtained by using the identity [16]

$$\int_0^\infty r^p e^{-r^2} dr = \frac{1}{2} \Gamma\left(\frac{1}{2}(p+1)\right). \quad (41)$$

The wavefunctions obtained are eigenfunctions of H with eigenvalues given by equation (33).

Wavefunctions for $n \neq 0$ states are obtained from the $n = 0$ states using the $\mathfrak{su}(1, 1)$ raising operators in accord with equation (13). In this way, one obtains radial wavefunctions that are analytic continuations of spherical harmonic oscillator functions and, like them, expressible in terms of associated Laguerre polynomials.

Apart from the reduced mass, the Hamiltonian H of equation (22) contains two adjustable parameters: ω and ε . The frequency ω can be set to give the energy $E_{10} = 2\hbar\omega$ of the first $l = 0$ vibrational state at its observed value. The parameter ε can be set equal to r_0^4 , where r_0 is the equilibrium separation of the two atoms.

For large values of ε , one can expand the expression for E_{nl} in inverse powers of ε to give

$$E_{nl} = E_0 + 2n\hbar\omega + Al(l+1) - Bl^2(l+1)^2 + \dots \quad (42)$$

with

$$A = \frac{\hbar\omega}{2\sqrt{\varepsilon}} \quad B = \frac{1}{4\varepsilon} A. \quad (43)$$

For example, for the HCl molecule, the first vibrational state is at energy $2\hbar\omega = 2885.9 \text{ cm}^{-1}$ and the inertia parameter has value $A = 10.437 \text{ cm}^{-1}$. Thus, we infer that ε should be given the value

$$\varepsilon = \left(\frac{\hbar\omega}{2A}\right)^2 = 4778 \quad (44)$$

and $B \approx 0.00055$. One sees that the Davidson potential predicts a ground-state rotational band for the HCl molecule that is extremely close to that of a rigid rotor as observed.

Electromagnetic transition rates between molecular states are easily computed in the model. Consider, for example, the dipole operators

$$D_{1k} = Ze r Y_{1k}(\theta, \varphi) \quad k = 0, \pm 1 \quad (45)$$

where Ze is the effective charge. With the wavefunctions of equation (39) and the identity of equation (41) we obtain the reduced matrix elements

$$\langle 0l-1 || D_1 || l \rangle = \sqrt{\frac{3l}{4\pi}} \frac{Ze \Gamma(\frac{1}{2}b_l + \frac{1}{2}b_{l-1} + 2)}{[\Gamma(b_l + \frac{3}{2})\Gamma(b_{l-1} + \frac{3}{2})]^{1/2}}. \quad (46)$$

Thus, the reduced dipole transition rates

$$B(E1; 0l \rightarrow 0, l-1) = \frac{|\langle 0l-1 || D_1 || l \rangle|^2}{(2l+1)} \quad (47)$$

take the values

$$B(E1; 0l \rightarrow 0, l-1) = \frac{3}{4\pi} Z^2 e^2 \frac{l}{2l+1} \cdot \frac{\Gamma(\frac{1}{2}b_l + \frac{1}{2}b_{l-1} + 2)^2}{\Gamma(b_l + \frac{3}{2})\Gamma(b_{l-1} + \frac{3}{2})}. \quad (48)$$

When $\varepsilon = 0$, this expression reduces to that of the spherical harmonic oscillator

$$B(E1; 0l \rightarrow 0, l-1)_{\text{SHO}} = \frac{3Z^2 e^2 l}{8\pi}. \quad (49)$$

Table 1. Some values of the ratio $R(l; \varepsilon)$. At $\varepsilon = 0$ the results are characteristic of a spherical (harmonic) vibrator while for large ε they approach rotor values.

$l \setminus \varepsilon$	0	5	10	20	∞
2	2.0	1.37	1.31	1.26	1.20
3	3.0	1.74	1.58	1.46	1.29
4	4.0	2.14	1.86	1.66	1.33
5	5.0	2.56	2.17	1.87	1.36

When $\varepsilon \rightarrow \infty$, we can use the identity [16]

$$\lim_{n \rightarrow \infty} n^{b-a} \frac{\Gamma(n+a)}{\Gamma(n+b)} = 1 \quad (50)$$

to obtain the rotor model expression

$$B(E1; 0l \rightarrow 0, l-1)_{\text{ROT}} = \frac{3}{4\pi} Z^2 e^2 \sqrt{\varepsilon} \frac{l}{2l+1} \quad (51)$$

for two atoms with separation distance $r_0 = \varepsilon^{1/4}$. From the values of the ratios

$$R(l; \varepsilon) = \frac{B(E1; 0l \rightarrow 0, l-1)_\varepsilon}{B(E1; 01 \rightarrow 00)_\varepsilon} \quad (52)$$

shown in table 1, one sees that $B(E1; 0l \rightarrow 0, l-1)_\varepsilon$ indeed changes rapidly with increasing ε from harmonic oscillator values to those of a rotor.

The HCl molecule, with $\varepsilon = 4778$ is evidently extremely close to the rigid rotor limit.

4. Many-particle systems with Davidson interactions

The Hamiltonian for A particles in three dimensions with Davidson interactions is given by

$$H = \frac{1}{2} \hbar \omega \sum_{n=1}^A \left[(-\nabla_n^2 + r_n^2) + \sum_{m \neq n} \frac{\varepsilon}{|\mathbf{r}_m - \mathbf{r}_n|^2} \right]. \quad (53)$$

This Hamiltonian has an $\mathfrak{sp}(1, \mathbb{R}) \sim \mathfrak{su}(1, 1)$ SGA with

$$\begin{aligned} \hat{Z}'_1 &= \hbar^2 \sum_n \left[-\nabla_n^2 + \sum_{m \neq 0} \frac{\varepsilon}{|\mathbf{r}_m - \mathbf{r}_n|^2} \right] & \hat{Z}'_2 &= \sum_n r_n^2 \\ \hat{Z}'_3 &= -\frac{1}{2} i \hbar \sum_n (\mathbf{r}_n \cdot \nabla_n + \nabla_n \cdot \mathbf{r}_n). \end{aligned} \quad (54)$$

It is $\text{SO}(3)$ and S_A invariant, where S_A is the symmetric group of permutations of the A -particle indices. Thus, H has energy levels given by

$$E_{n\alpha L} = [2n + \lambda(\alpha L)] \hbar \omega. \quad (55)$$

This equation shows that the relative energies of states within an $\mathfrak{su}(1, 1)$ irrep follow a harmonic oscillator sequence. We have not been able to determine the lowest weights $\{\lambda(\alpha L)\}$ for the many $\mathfrak{su}(1, 1)$ irreps that occur. Consequently, we do not know the relative energies of states belonging to different $\mathfrak{su}(1, 1)$ irreps. Thus, it appears that the Hamiltonian (53) is only partially integrable.

To determine the lowest weights $\{\lambda(\alpha L)\}$, and hence the low-energy spectrum for the Hamiltonian of equation (53), it would appear that we need to proceed numerically. However, to do so requires the construction of a suitable basis in terms of which expansions

of the desired eigenstates would be rapidly convergent. The search for such a basis presents a challenge we have not resolved.

It is of interest to note that in one dimension the Hamiltonian for a many-particle system with Davidson interactions

$$H = \frac{1}{2}\hbar\omega \sum_n \left[\left(-\frac{d^2}{dx_n^2} + x_n^2 \right) + \sum_{m \neq n} \frac{\varepsilon}{|x_m - x_n|^2} \right] \quad (56)$$

is the Hamiltonian of the Calogero model [8]. This Hamiltonian is known to have a subset of analytical solutions [8, 17]. Thus, it is appropriate to consider their structure to see if they can extend to three dimensions.

If $r^2 = \sum_{n=1}^A x_n^2$, then the eigenfunctions of the Hamiltonian (56), with the correct boundary conditions, are of the form

$$\psi(x) = P(x)e^{-r^2/2\alpha} \quad \alpha = \frac{m\omega}{\hbar} \quad (57)$$

where P is a polynomial in the variables $x = (x_1, \dots, x_A)$. Using the identity

$$\frac{\partial}{\partial x_n} e^{-r^2/2\alpha} = e^{-r^2/2\alpha} \left(\frac{\partial}{\partial x_n} - \frac{x_n}{\alpha} \right) \quad (58)$$

one finds that P satisfies the eigenfunction equation

$$\sum_n \left[\left(-\frac{\partial^2}{\partial x_n^2} + x_n \frac{\partial}{\partial x_n} + \frac{\partial}{\partial x_n} x_n \right) + \sum_{m \neq n} \frac{\varepsilon}{|x_n - x_m|^2} \right] P(x) = \frac{2E}{\hbar\omega} P(x). \quad (59)$$

Calogero showed that if z is the Vandermonde determinant

$$z = \prod_{n < m} (x_n - x_m) \quad (60)$$

then

$$\sum_n \frac{\partial z}{\partial x_n} = \sum_n \frac{\partial^2 z}{\partial x_n^2} = 0 \quad (61)$$

and

$$\sum_n \left(\frac{\partial z}{\partial x_n} \right)^2 = z^2 \sum_n \sum_{m \neq n} \frac{1}{(x_n - x_m)^2}. \quad (62)$$

It follows that a solution to equation (59) is obtained with

$$P(x) = z^a \quad (63)$$

where

$$a = \frac{1}{2} + \frac{1}{2}\sqrt{1 + 4\varepsilon} \quad \text{for } \varepsilon \neq 0 \quad (64)$$

and

$$E = \frac{1}{4}A(A-1) \left[1 + \sqrt{1 + 4\varepsilon} \right] \hbar\omega. \quad (65)$$

Unfortunately, it does not appear that the eigenfunctions of the Calogero Hamiltonian obtained in this way extend to the corresponding three-dimensional problem. If they did, they would not be the wavefunctions normally chosen for a many-fermion system because, although $\psi(x)$, defined by equations (57) and (63), obeys an exclusion principle, it is not antisymmetric (neither is it symmetric).

5. The nuclear collective model

If the $\{q_v\}$ coordinates of the nuclear collective model (CM) are expressed in the standard way [9]

$$q_v = \beta \cos \gamma \mathcal{D}_{0v}^2(\Omega) + \frac{1}{\sqrt{2}} \beta \sin \gamma (\mathcal{D}_{2v}^2(\Omega) + \mathcal{D}_{-2v}^2(\Omega)) \quad (66)$$

in terms of intrinsic (β, γ) coordinates and rotational $\Omega \in \text{SO}(3)$ angles, the quadrupole Davidson potential acquires the simple form

$$V(\beta) = \frac{1}{2} B \omega^2 \left(q \cdot q + \frac{\varepsilon}{q \cdot q} \right) = \frac{1}{2} B \omega^2 \left(\beta^2 + \frac{\varepsilon}{\beta^2} \right). \quad (67)$$

As for the diatomic molecule, we can simplify the notation further by putting the coordinates in harmonic oscillator units. In these units $\hbar/B\omega \rightarrow 1$ and the Hamiltonian (3) becomes

$$H_\varepsilon = \frac{1}{2} \hbar \omega \left(-\nabla^2 + \beta^2 + \frac{\varepsilon}{\beta^2} \right) \quad (68)$$

where ∇^2 is the Laplacian operator in the five-dimensional space of the model.

Both ∇^2 and $\beta^2 = q \cdot q$ are scalar products of five-component vectors. Thus, the Hamiltonian H_ε is $\text{SO}(5)$ invariant. Such Hamiltonians for the CM have been considered by Wilets and Jean [10]. They are characterized by the fact that their potentials are functions only of β ; they are independent of γ and Ω (the latter due to $\text{SO}(3)$ invariance) and are often described as being γ -soft. The additional feature of the collective Hamiltonian with a Davidson potential is that, as well as having an $\text{SO}(5)$ symmetry group, it also has an $\text{SU}(1, 1)$ dynamical group.

It is known (cf [18]) that an orthonormal basis for the CM is given by a set of states $\{|n\nu\alpha LM\rangle\}$ labelled by quantum numbers of the subgroup chain

$$\begin{array}{ccccccc} \text{SU}(1, 1) \times \text{SO}(5) & \supset & \text{U}(1) \times \text{SO}(3) & \supset & \text{SO}(2) & & \\ \lambda & & \nu & \alpha & n & L & M \end{array} \quad (69)$$

where λ is an $\text{SU}(1, 1)$ lowest weight, ν (the so-called $\text{SO}(5)$ seniority) is the highest weight for an $\text{SO}(5)$ irrep and α indexes the $\text{SO}(3)$ multiplicity.

The energy level spectrum for the $\varepsilon = 0$ Hamiltonian H_0 is the harmonic vibrational spectrum for which

$$\lambda(\varepsilon = 0) = \nu + \frac{5}{2} \quad (70)$$

and

$$E_{n\nu}(\varepsilon = 0) = (2n + \nu + \frac{5}{2}) \hbar \omega \quad (71)$$

with $\nu = 0, 1, 2, \dots$ and $n = 0, 1, 2, \dots$. Each $(n\nu)$ pair indexes a multiplet of states which span a corresponding $\text{SO}(5)$ irrep of highest weight ν . Such an irrep comprises a range of $\text{SO}(3)$ states given [19] by

$$\begin{aligned} L &= 2K, 2K - 2, 2K - 3, \dots, K \\ K &= \nu, \nu - 3, \nu - 6, \dots, \nu \\ \nu &= 0, 1, \text{ or } 2. \end{aligned} \quad (72)$$

To obtain the energy levels of H_ε we define

$$\begin{aligned} \hat{Z}_1 &= -\hbar^2 \nabla^2 & \hat{Z}_2 &= \beta^2 \\ \hat{Z}_3 &= -\frac{1}{2} i \hbar (q \cdot \nabla + \nabla \cdot q). \end{aligned} \quad (73)$$

and, for $\varepsilon \neq 0$, make the nonlinear transformation

$$\hat{Z}'_1 = \hat{Z}_1 + \frac{\hbar^2 \varepsilon}{\hat{Z}_2} \quad \hat{Z}'_2 = \hat{Z}_2 \quad \hat{Z}'_3 = \hat{Z}_3. \quad (74)$$

Both the $\{\hat{Z}_i\}$ and $\{\hat{Z}'_i\}$ operators then satisfy the $\mathfrak{sp}(1, \mathbb{R}) \sim \mathfrak{su}(1, 1)$ commutation relations of equation (9). Thus, we transform to $\{\hat{X}_i\}$ operators by means of equation (11) and, setting $a = 1/B\omega$, obtain

$$H_\varepsilon = 2\hbar\omega\hat{X}_0. \quad (75)$$

It follows that the energy-level spectrum of H_ε is given by

$$E_{nv} = [2n + \lambda(v)]\hbar\omega. \quad (76)$$

To determine $\lambda(v)$ when $\varepsilon \neq 0$, we again consider the expression for the $\mathfrak{su}(1, 1)$ Casimir operator

$$\mathbb{C}_2 = \mathbb{C}_2(\varepsilon = 0) + \frac{1}{4}\varepsilon. \quad (77)$$

It follows now from equation (70) that

$$\lambda(v)(\lambda(v) - 2) = (v + \frac{5}{2})(v + \frac{1}{2}) + \varepsilon \quad (78)$$

and

$$\lambda(v) = 1 + \sqrt{(v + \frac{3}{2})^2 + \varepsilon}. \quad (79)$$

Thus, we obtain the energy-level spectrum

$$E_{nv}(\varepsilon) = \left[2n + 1 + \sqrt{(v + \frac{3}{2})^2 + \varepsilon} \right] \hbar\omega. \quad (80)$$

For $\varepsilon = 0$, we regain the harmonic vibrational limit of equation (71). For large values of ε , we obtain

$$E_{nv}(\varepsilon) = E_0 + 2n\hbar\omega + \frac{\hbar\omega}{2\sqrt{\varepsilon}}v(v+3) + \dots \quad (81)$$

which, for $\varepsilon \rightarrow \infty$ and $\hbar\omega \rightarrow \infty$, gives the characteristic spectrum of the β -rigid, γ -soft limit of the CM;

$$E_v = E_0 + Av(v+3). \quad (82)$$

However, we also obtain a complete range of solutions for finite values of ε . Some examples are shown in figure 1.

Wavefunctions for the $\mathfrak{su}(1, 1)$ lowest weight states $\{|0v\alpha LM\rangle\}$ can be expressed

$$\Psi_{\alpha LM}^v(q) = e^{-\beta^2/2} P_{\alpha LM}^v(q). \quad (83)$$

Since

$$\begin{aligned} \hat{X}_- e^{-\beta^2/2} &= \frac{1}{4} e^{-\beta^2/2} \left[-\nabla^2 + \frac{\varepsilon}{\beta^2} \right] \\ \hat{X}_0 e^{-\beta^2/2} &= \frac{1}{4} e^{-\beta^2/2} \left[-\nabla^2 + \frac{\varepsilon}{\beta^2} + q \cdot \nabla + \nabla \cdot q \right] \end{aligned} \quad (84)$$

and $\hat{X}_- \Psi_{\alpha LM}^v = 0$, it follows that

$$\hat{X}_0 \Psi_{\alpha LM}^v(q) = \frac{1}{4} e^{-\beta^2/2} [2q \cdot \nabla + 5] P_{\alpha LM}^v(q). \quad (85)$$

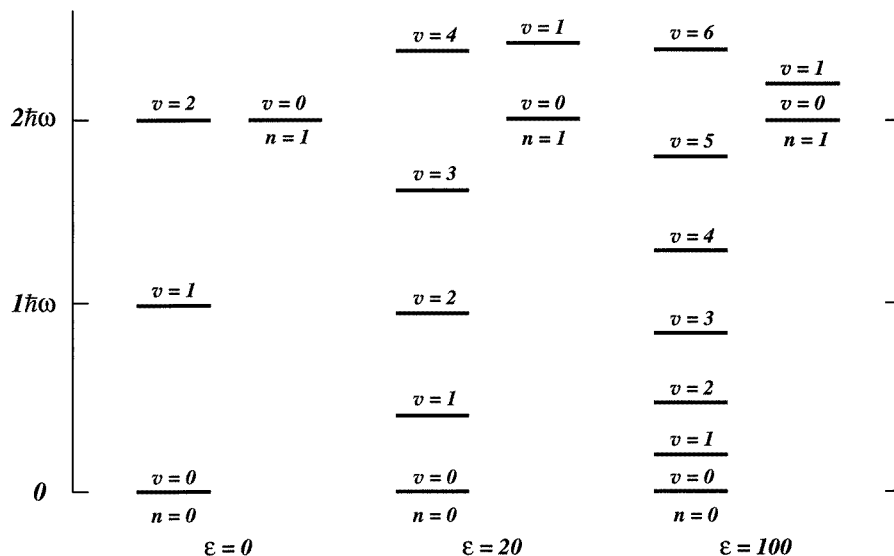


Figure 1. Energy-level spectra for the collective model for selected values of ε .

We also know from the energy spectrum that

$$\hat{X}_0 \Psi_{\alpha LM}^v(q) = \frac{1}{2} \lambda(v) \Psi_{\alpha LM}^v(q). \tag{86}$$

It follows that $P_{\alpha LM}^v$ is a polynomial of degree

$$b_v = \lambda(v) - \frac{5}{2} = \sqrt{(v + \frac{3}{2})^2 + \varepsilon} - \frac{3}{2}. \tag{87}$$

When $\varepsilon = 0$, the polynomials are solutions of Laplace’s equation; $\nabla^2 P_{\alpha LM}^v = 0$. Thus, they are harmonic polynomials;

$$P_{\alpha LM}^v(q) \xrightarrow{\varepsilon=0} \beta^v \mathcal{Y}_{\alpha LM}^v(\zeta) \tag{88}$$

where $\mathcal{Y}_{\alpha LM}^v$ is an SO(5) spherical harmonic and ζ is a suitable set of spherical coordinates for the unit SO(5) sphere. For arbitrary ε the wavefunctions are then

$$\Psi_{\alpha LM}^v(q) = N_v e^{-\beta^2/2} \beta^{b_v} \mathcal{Y}_{\alpha LM}^v(\zeta) \tag{89}$$

where N_v is a norm factor.

Wavefunctions for $n \neq 0$ states are obtained from the $n = 0$ states using the $\mathfrak{su}(1, 1)$ raising operators in accord with equation (13). In this way, one obtains wavefunctions that are analytic continuations of spherical vibrator functions and, like them, expressible in terms of associated Laguerre polynomials in β [11].

We now consider predictions of the model for electromagnetic quadrupole transitions. Assuming the quadrupole transition operators to be of the form

$$Q_v = k\beta Y_{2v} \tag{90}$$

where k is a constant, and the volume element of the collective model to be of the form $\beta^4 d\beta dv(\zeta)$, where $dv(\zeta)$ is the SO(5) invariant measure, the required matrix elements for the ground-state band of $n = 0$ states are given by the expression

$$\langle 0v'\alpha'L' \| Q \| 0v\alpha L \rangle = N_{v'} N_v \int_0^\infty e^{-\beta^2} \beta^{b_v+b_{v'}+5} d\beta k \langle \mathcal{Y}_{\alpha'L'}^{v'} \| Y_2 \| \mathcal{Y}_{\alpha L}^v \rangle. \tag{91}$$

Thus, we obtain

$$\langle 0v-1, \alpha' L' \| Q \| 0v\alpha L \rangle = k \langle \mathcal{Y}_{\alpha' L'}^{v-1} \| Y_2 \| \mathcal{Y}_{\alpha L}^v \rangle \frac{\Gamma(\frac{1}{2}(b_v + b_{v-1}) + 3)}{\sqrt{\Gamma(b_v + \frac{5}{2})\Gamma(b_{v-1} + \frac{5}{2})}}. \quad (92)$$

The $\langle \mathcal{Y}_{\alpha' L'}^{v-1} \| Y_2 \| \mathcal{Y}_{\alpha L}^v \rangle$ reduced matrix elements depend only on the properties of the SO(5) irreps involved. They can be evaluated by the methods given in [18].

The general expression for a quadrupole matrix element can also be obtained in terms of the corresponding expressions for the spherical vibrational limit of the CM, for which $\varepsilon = 0$. In the $\varepsilon = 0$ limit, the non-zero matrix elements are given by

$$\langle 0v-1, \alpha' L' \| Q \| 0v\alpha L \rangle_0 k \langle \mathcal{Y}_{\alpha' L'}^{v-1} \| Y_2 \| \mathcal{Y}_{\alpha L}^v \rangle \sqrt{v + \frac{3}{2}}. \quad (93)$$

Thus, we obtain

$$\frac{\langle 0v-1, \alpha' L' \| Q \| 0v\alpha L \rangle_\varepsilon}{\langle 0v-1, \alpha' L' \| Q \| 0v\alpha L \rangle_0} = \frac{\Gamma(\frac{1}{2}(b_v + b_{v-1}) + 3)}{\sqrt{(v + \frac{3}{2})\Gamma(b_v + \frac{5}{2})\Gamma(b_{v-1} + \frac{5}{2})}}. \quad (94)$$

The beta-rigid limit is obtained by taking the limit $\varepsilon \rightarrow \infty$ in which

$$b_v \rightarrow \sqrt{\varepsilon} - \frac{3}{2} \quad \frac{\Gamma(\sqrt{\varepsilon} + \frac{3}{2})}{\Gamma(\sqrt{\varepsilon} + 1)} \rightarrow \varepsilon^{\frac{1}{4}} = \beta_0 \quad (95)$$

where β_0 is the value of β for which the Davidson potential is a minimum. We obtain

$$\frac{\langle 0v-1, \alpha' L' \| Q \| 0v\alpha L \rangle_\infty}{\langle 0v-1, \alpha' L' \| Q \| 0v\alpha L \rangle_0} = \frac{\beta_0}{\sqrt{v + \frac{3}{2}}}. \quad (96)$$

6. Generalizations of the model

A limitation of the Davidson potential for applications in nuclear physics is that it is completely gamma-soft; it depends only on β . As a consequence the spectrum of the model given by equation (80) depends only the SO(5) seniority quantum number v , i.e. the angular momentum states within a given SO(5) irrep have the same energy.

An interesting potential to consider would be one which depends on both β and γ , e.g.

$$V(\beta, \gamma) = \frac{1}{2} B \omega^2 \left(q \cdot q + \frac{\varepsilon}{q \cdot q} \right) + \chi (q \times q \times q)^0 \quad (97)$$

where it is noted (from equation (66)) that

$$(q \times q \times q)^0 \sim \beta^3 \cos 3\gamma. \quad (98)$$

Such a potential would describe the coupled rotations and vibrations of a model nucleus with β - and γ -stiff but not rigid for finite values of ε and χ . Unfortunately, such a Hamiltonian is not diagonalized by states which reduce any known subalgebra chain. Thus, to determine the spectrum of the Hamiltonian of equation (97), it would be necessary to proceed numerically. However, one could expect to obtain much more rapidly convergent results in an $\varepsilon \neq 0$, SO(5) basis than in the spherical harmonic ($\varepsilon = 0$) basis customarily used [20] for CM calculations.

A quick and easy way to lift the degeneracy of states of an SO(5) multiplet would be to simply add a term to the Hamiltonian proportional to the SO(3) Casimir invariant $AL \cdot L$. Note that the $\mathfrak{so}(5)$ Lie algebra is spanned by three components of the angular momentum

and seven components of a (positive parity) octupole tensor O . Furthermore, the second order Casimir operator for $SO(5)$ is given (to within a constant numerical factor) by

$$\hat{C}_2^{so(5)} = O \cdot O + \frac{1}{10} \mathbf{L} \cdot \mathbf{L}. \tag{99}$$

Thus, to split the degeneracy of the $SO(5)$ multiplets, one could, equivalently, add an $O \cdot O$ interaction to the Hamiltonian, in parallel with the $Q \cdot Q$ interaction used in the $SU(3)$ model [21]. By either device, one simply adjusts the energies of states without changing their wavefunctions or matrix elements.

7. The symplectic model

The model Hamiltonians in three and five dimensions considered in the preceding sections are solvable by virtue of their $Sp(1, \mathbb{R})$ dynamical symmetries and their invariance under $SO(3)$ and $SO(5)$, respectively. However, for a many-particle system in three dimensions, we need additional symmetry. First observe that the quadrupole moments defined by equation (4) are linear combinations of the Cartesian scalar products of A -component vectors

$$Q_{ij} = \sum_{n=1}^A x_{ni} x_{nj} \tag{100}$$

where (x_{n1}, x_{n2}, x_{n3}) are Cartesian coordinates for the n th particle. Thus, the quadrupole moments are scalars under orthogonal $O(A)$ transformations in particle-index space. It follows that the scalar product $Q \cdot Q$ and the potential $V(Q)$ of equation (5) are invariant under both $SO(3)$ and $O(A)$. We therefore consider the many-particle Hamiltonian

$$H = \frac{1}{2} \hbar \omega \sum_n (-\nabla_n^2 + r_n^2) + \chi \left(Q \cdot Q + \frac{\varepsilon}{Q \cdot Q} \right). \tag{101}$$

In replacing $\sum_n r_n^2$ by $Q \cdot Q$ in the Davidson potential, the $Sp(1, \mathbb{R})$ dynamical symmetry is lost. However, the larger dynamical symmetry $Sp(3, \mathbb{R})$ remains. The essential observation is that the Hamiltonian (101) is a function of the elements

$$\begin{aligned} K_{ij} &= \sum_n p_{ni} p_{nj} & Q_{ij} &= \sum_n x_{ni} x_{nj} \\ P_{ij} &= \frac{1}{2} \sum_n (x_{ni} p_{nj} + p_{nj} x_{ni}) \end{aligned} \tag{102}$$

of an $\mathfrak{sp}(3, \mathbb{R})$ Lie algebra. Thus, the Hamiltonian (101) leaves the carrier space for an $\mathfrak{sp}(3, \mathbb{R})$ irrep invariant.

It may be noted that the group $Sp(3, \mathbb{R})$ contains $SO(3)$ as a subgroup and its elements all commute with those of $O(A)$. Thus, $Sp(3, \mathbb{R})$ takes full advantage of the $SO(3) \times O(A)$ invariance of the Hamiltonian.

Unfortunately, we no longer have a chain of dynamical subgroups which would enable us to deduce the spectrum and eigenfunctions of the Hamiltonian by purely algebraic methods. However, the $Sp(3, \mathbb{R})$ dynamical symmetry makes it possible to determine the spectrum and eigenfunctions of the Hamiltonian on a computer.

The calculations can be carried out in a basis for an $Sp(3, \mathbb{R})$ irrep that reduces the $SU(3) \subset Sp(3, \mathbb{R})$ subgroup. The many-particle harmonic oscillator part of H is diagonal in this basis. The added Davidson potential is not diagonal but its matrix elements are easily computed. Efficient methods for computing $\mathfrak{sp}(3, \mathbb{R})$ matrix elements and diagonalizing Hamiltonians in the $\mathfrak{sp}(3, \mathbb{R})$ enveloping algebra have been developed and are discussed

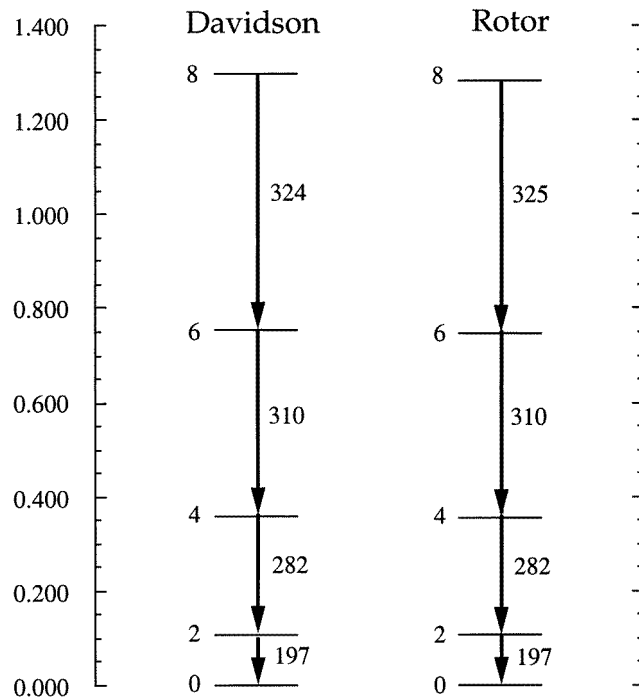


Figure 2. Energy-level spectrum for the symplectic model compared to that for the rigid rotor model. The angular momentum L values are given on the left of each energy level and the reduced quadrupole transition $B(E2)$ are given between two levels, next to the transition arrows.

elsewhere [13–15]. These methods make maximal use of the $SU(3)$ -coupling coefficient technology of Draayer and Akiyama [22].

A fuller analysis of the symplectic model with a Davidson potential will be presented in a following paper. We present here some preliminary results to show the kind of spectrum and reduced quadrupole transition rates that can be obtained. The calculation is for a mass $A = 166$ nucleus. The oscillator strength is set such that $\hbar\omega = 7.46$ MeV which is reasonable for such a nucleus. The parameters ε and χ are adjusted to give an appropriate energy difference between the $L = 0$ and $L = 2$ states. As it can be seen from figure 2, the spectrum closely resembles that of a rigid rotor, shown for comparison, for which the energies are proportional to $L(L + 1)$ and the $B(E2)$ values are proportional to the squares of Clebsch–Gordan coefficients [9].

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