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An $su(1,1)$ dynamical algebra for the Morse potential

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Abstract
An $su(1,1)$ dynamical algebra to describe both the discrete and the continuum parts of the spectrum for the Morse potential is proposed. The space associated with this algebra is given in terms of a family of orthonormal functions $\{\Phi_n^\sigma\}$ characterized by the parameter σ. This set is constructed from polynomials which are orthogonal with respect to a weighting function related to a Morse ground state. An analysis of the associated algebra is investigated in detail. The functions are identified with Morse-like functions associated with different potential depths. We prove that for a particular choice of σ the discrete and the continuum parts of the spectrum decouple. The connection of this treatment with the supersymmetric quantum mechanics approach is established. A closed expression for the Mecke dipole moment function is obtained.

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1. Introduction

New experimental techniques based on lasers have allowed us to develop research in energy regions where chemical activity becomes significant [1]. In particular, stimulated emission pumping (SEP) spectroscopy and disperse fluorescence (DF) spectroscopy [2, 3] have been widely used to study energy intramolecular vibrational redistribution, which represents a physical process of significant importance to characterize the possible reaction pathways [4, 5]. The activation chemical reactivity implies dealing with breaking of molecular bonds to produce a new rearrangement of atoms or even a dissociation process. In the description of these phenomena the continuum part of the spectrum plays a preponderant role and consequently it must be taken into account in any theoretical framework. Due to its importance, great attention has been paid to incorporate the continuum, appropriately discretized, in the description of the system [6–17].

Models based on a harmonic basis of the vibrational degrees of freedom are clearly unsuitable, since a breakup threshold is non-existent in these models. This problem is overcome by the local models developed in the last three decades, where the vibrational excitations are described by means of a set of interacting local oscillators associated with local coordinates [18–22]. In these models the stretching vibrations are described by Morse potentials, which incorporate the main characteristics of real diatomic systems, namely, anharmonicity and dissociation [23]. This potential has the additional advantage of belonging to the solvable-potential family, and consequently many analytical results can be used [24, 25]. However, most of the studies using Morse oscillators consider just the bound part of the spectrum [19–32]. Here, we propose a method for treating both the bound and the unbound parts of the Morse spectrum on an equal footing.

In this work we present a complete basis for the Morse oscillator, which is given by a set of orthogonal polynomials with respect to a weighting function determined from a Morse ground state. This approach provides a family of suitable complete orthogonal bases to incorporate both the bound and continuum states, and has the advantage that by choosing appropriately the set of functions it is possible to decouple the discrete from the continuum part of the spectrum. In addition, the Hamiltonian representation turns out to be tridiagonal, a fact of practical consequences. This basis has already been proposed to describe the continuum using different arguments based on supersymmetric quantum mechanics [33, 34].

The description of the Morse potential in terms of the proposed orthonormal basis can be done in configuration space [16]. In this work we intend to establish an algebraic approach to the problem. We establish the dynamical algebra generated by the basis. We show how this identification allows us to obtain analytical formulae for the matrix elements of different relevant operators, in particular those corresponding to the dipole moment. In section 2 the basis is obtained as well as the associated raising and lowering operators, which are shown to satisfy the $su(1,1)$ commutation relations. Section 3 is devoted to the analysis of the Morse Hamiltonian. In section 4 an interpretation of the proposed basis is provided. In section 5 the calculation of the matrix elements for the Mecke dipole moment function is included. Finally, in section 6 the summary and conclusions are presented.

2. An orthonormal complete basis for the Morse potential

We start by establishing the bound solutions for the Morse potential. Choosing the limit of the separated atoms as the zero of energy, the Morse potential has the following form [23]:

$$V(x) = D(\mathrm{e}^{-2\beta x} - 2\,\mathrm{e}^{-\beta x}) \tag{1}$$

where $D > 0$ corresponds to its depth, β is related to the range of the potential and x gives the relative distance from the equilibrium position of the atoms.

The solution of the Schrödinger equation associated with the potential (1) is given by [23]

$$\Psi_v^j(y) = N_v^j\,\mathrm{e}^{-\frac{y}{2}}y^{j-v}L_v^{2(j-v)}(y) \tag{2}$$

where $L_n^s(y)$ are the associated Laguerre functions, the argument y is related to the physical displacement coordinate x by $y = (2j+1)\,\mathrm{e}^{-\beta x}$, N_v^j is the normalization constant

$$N_v^j = \sqrt{\frac{\beta(2j-2v)\Gamma(v+1)}{\Gamma(2j-v+1)}} \tag{3}$$

where v is a non-negative integer and j is a real positive value. They are related to the potential and energy through

$$2j+1 = \sqrt{\frac{8\mu D}{\beta^2\hbar^2}} \qquad j-v = \sqrt{\frac{-2\mu E}{\beta^2\hbar^2}} \tag{4}$$

where μ is the reduced mass of the molecule. Normalizable states fulfil $v < j$ and the corresponding energy spectrum is

$$E_v = -\hbar\omega(v - j)^2 \tag{5}$$

where

$$\omega = \frac{\hbar\beta^2}{2\mu}. \tag{6}$$

It is possible to obtain an algebraic representation of the solutions (2) by introducing creation $\hat{b}^\dagger$ and annihilation $\hat{b}$ operators [29], which have the following action on the functions (2):

$$\hat{b}^\dagger \Psi_v^j(y) = \sqrt{(v+1)(1-(v+1)/(2j+1))}\,\Psi_{v+1}^j(y) \tag{7a}$$

$$\hat{b}\Psi_v^j(y) = \sqrt{v(1-v/(2j+1))}\,\Psi_{v-1}^j(y) \tag{7b}$$

with

$$\hat{v}\Psi_v^j(y) = v\Psi_v^j(y). \tag{8}$$

The operators $\{b^\dagger, b\}$ actually depend on j and v, which means that they are defined only in the space of solutions (2). To simplify the notation, however, we prefer not to introduce this dependence explicitly. A similar situation occurs with the variable y, which depends on j and β.

The operators $\{b^\dagger, b\}$, together with the number operator $\hat{v}$, satisfy the commutation relations

$$[\hat{b}, \hat{b}^\dagger] = 1 - \frac{2\hat{v}+1}{(2j+1)} \qquad [\hat{v}, \hat{b}^\dagger] = \hat{b}^\dagger \qquad [\hat{v}, \hat{b}] = -\hat{b} \tag{9}$$

which can be identified with the usual $su(2)$ commutation relations by introducing the set of transformations $\{b^\dagger = \hat{J}_-/\sqrt{(2j+1)},\quad b = \hat{J}_+/\sqrt{(2j+1)},\quad \hat{v} = j - \hat{J}_0\}$, where J_μ satisfy the usual 'angular momentum' commutation relations [35]. The $su(2)$ group is the dynamical symmetry for the bound states for the Morse potential and any dynamical variable can be expanded in terms of the generators

$$G_{su(2)} = \{\hat{b}^\dagger, \hat{b}, \hat{v}\}. \tag{10}$$

The projection of the angular momentum m is related to v by [36]

$$m = v - j. \tag{11}$$

From this relation we see that the ground state ($v = 0$) corresponds to $m = -j$. The states corresponding to $v \geqslant j$, however, are not normalizable, and consequently

$$v_{\max} = [j] \tag{12}$$

where the notation $[j]$ stands for the closest integer to j that is smaller than j. We shall thus consider Morse potentials with $[j] + 1$ bound states. In the algebraic space the functions (2) acquire the simple form

$$\left|\Psi_v^j\right\rangle = \mathcal{N}_v^j (\hat{b}^\dagger)^v \left|\Psi_0^j\right\rangle \tag{13}$$

with normalization constant

$$\mathcal{N}_v^j = \sqrt{(2j+1)^v \frac{\Gamma(2j-v+1)}{v!\,\Gamma(2j+1)}}. \tag{14}$$

The Morse functions are then associated with one branch (in this case with $m < 0$) of the $su(2)$ representations. It is important to remark that in the $su(2)$ space the Morse variable

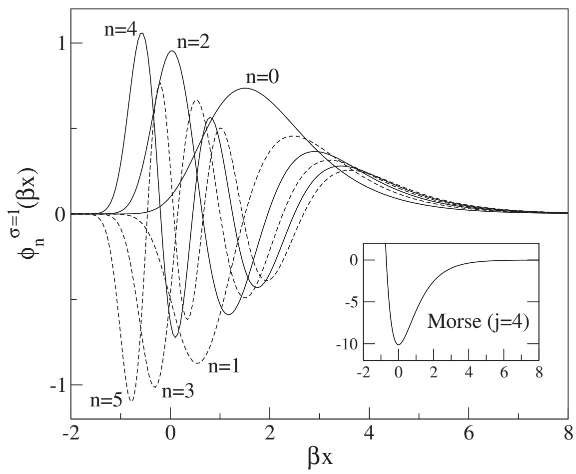

Figure 1. $N = 6$ basis for the Morse potential for the case $\sigma = 1$ (βx is dimensionless). In the inset a Morse potential with $j = 4$ (energy given in units of $\hbar^2\beta^2/\mu$) is represented.

y, the coordinate x and the momentum p take the form of a finite expansion in the parameter $1/\sqrt{(2j+1)}$ involving all allowed powers of the generators [31].

The bound solutions (2) do not form a complete set of states in the Hilbert space. A complete set is obtained when the continuum part of the spectrum is taken into account. Instead of considering the analytic solutions for the continuous part of the spectrum we shall introduce a continuum discretization by means of a complete set of orthonormal functions. We propose the following set of functions:

$$\Phi_n^\sigma(y) = A_n^\sigma L_n^{2\sigma-1}(y) y^\sigma \,\mathrm{e}^{-y/2} \qquad n = 0, 1, 2, \ldots \tag{15}$$

with normalization constant

$$A_n^\sigma = \sqrt{\frac{\beta n!}{\Gamma(2\sigma + n)}}. \tag{16}$$

The family of functions (15) constitutes complete orthonormal sets $\mathcal{L}_\sigma$, each of them characterized by σ in the space $L^2[(0,\infty), \mathrm{d}y/y]$(the square integrable functions on the $(0,\infty)$ interval, with respect to the measure $\mathrm{d}y/y$). The proof that this family of functions is a complete set is given, for instance, in [37] in which it is demonstrated that the system $x^{a/2}\,\mathrm{e}^{-x/2} L_n^a(x)$ is closed in $L^2(0, +\infty)$ which is equivalent to saying that the system (15) is closed and consequently complete in $L^2[(0,\infty), \mathrm{d}y/y]$. In principle we can choose any possible σ to describe the Morse states. We shall show however that a particular σ allows us to split the bound states from the continuum part of the spectrum.

Once a value of σ is selected the infinite set (15) is complete, however in actual calculations the basis is truncated. The procedure will be useful if the number of states to be considered to provide a good approximation to the converged results for relevant observables is small enough. In section 5 some of these convergence tests for the basis proposed are presented.

In figure 1 the first few basis wavefunctions for the selection $\sigma = 1$ are plotted as functions of the dimensionless quantity βx, taking a basis of $N = 6$ functions. In the next section we will use this basis to diagonalize the Morse Hamiltonian and will present some results for the case $j = 4$ as an example. In the inset to figure 1 this Morse potential is plotted (energies are given in units of $\hbar^2\beta^2/\mu$). It can be seen that the basis wavefunctions explore distances out of the range of the potential.

For the time being we shall consider σ as a free parameter. The Morse Hamiltonian can now be diagonalized in the basis (15) to generate both the discrete and continuum parts of the spectrum. Although this task can be achieved in configuration space [16], we shall follow an algebraic procedure similar to that followed in the case of the bound states [29].

In accordance with the factorization method [38, 39], we proceed to obtain the ladder operators for the orthonormalized basis. To this end we start by establishing the action of the differential operator $\frac{\mathrm{d}}{\mathrm{d}y}$ on the functions (15):

$$\frac{\mathrm{d}}{\mathrm{d}y}\Phi_n^\sigma(y) = \left(\frac{\sigma}{y} - \frac{1}{2}\right)\Phi_n^\sigma(y) + A_n^\sigma y^\sigma \,\mathrm{e}^{-y/2}\frac{\mathrm{d}}{\mathrm{d}y}L_n^{2\sigma-1}(y). \tag{17}$$

Taking into account the recurrence relations [40]

$$y\frac{\mathrm{d}}{\mathrm{d}y}L_n^k(y) = nL_n^k(y) - (n+k)L_{n-1}^k(y) \tag{18}$$

$$-(n+k)L_{n-1}^k(y) = (n+1)L_{n+1}^k(y) - (2n+k+1-y)L_n^k(y) \tag{19}$$

we can define the rising, lowering and number operators

$$\hat{K}_- = -y\frac{\mathrm{d}}{\mathrm{d}y} - \frac{y}{2} + (\sigma + \hat{n}) \tag{20a}$$

$$\hat{K}_+ = y\frac{\mathrm{d}}{\mathrm{d}y} - \frac{y}{2} + (\sigma + \hat{n}) \tag{20b}$$

$$\hat{K}_0 = \sigma + \hat{n} = -y\frac{\mathrm{d}^2}{\mathrm{d}y^2} + \frac{y}{4} + \frac{\sigma(\sigma-1)}{y} \tag{20c}$$

with the following effect over the basis wavefunctions (15):

$$\hat{K}_-\Phi_n^\sigma(y) = k_-\Phi_{n-1}^\sigma(y) \qquad \text{with} \quad k_- = \sqrt{n(2\sigma+n-1)}. \tag{21a}$$

$$\hat{K}_+\Phi_n^\sigma(y) = k_+\Phi_{n+1}^\sigma(y) \qquad \text{with} \quad k_+ = \sqrt{(n+1)(2\sigma+n)}. \tag{21b}$$

$$\hat{K}_0\Phi_n^\sigma(y) = k_0\Phi_n^\sigma(y) \qquad \text{with} \quad k_0 = \sigma + n. \tag{21c}$$

As we can see, the operator $\hat{K}_-$ annihilates the ground state $\Phi_0^\sigma(y)$, as expected from a step-down operator. In equations (20*a*)–(20*c*) the operator $\hat{n}$ is to be understood as a diagonal operator

$$\hat{n}\Phi_n^\sigma = n\Phi_n^\sigma \tag{22}$$

similar to equation (8).

$\hat{K}_0$ together with the operators $\hat{K}_\pm$ satisfies the commutation relations

$$[\hat{K}_+, \hat{K}_-] = -2\hat{K}_0 \qquad [\hat{K}_0, \hat{K}_-] = -\hat{K}_- \qquad [\hat{K}_0, \hat{K}_+] = \hat{K}_+ \tag{23}$$

which correspond to the $su(1, 1)$ algebra [41]. We now proceed to identify the quantum numbers $\{\sigma, n\}$ according to the standard representation [42]. The latter is found by examining the formulae for the $su(1, 1)$ discrete series representation.

The $SU(1, 1)$ group is noncompact [41]. Unlike the case of $SU(2)$ all its unitary irreducible representations are infinite dimensional, and can be classified into three different kinds, the principal (continuous), discrete and supplementary series [42, 43]. In this work we shall be concerned only with the discrete series since the basis we are considering is discrete. The $SU(1, 1)$ generators $\hat{K}_{\pm,0}$ satisfy the commutation relations (23) and the discrete representations D_κ^+ of this group have the standard form

$$\hat{K}_+|\kappa, m\rangle = \sqrt{(m+\kappa)(m-\kappa+1)}|\kappa, m+1\rangle \tag{24a}$$

$$\hat{K}_-|\kappa, m\rangle = \sqrt{(m-\kappa)(m+\kappa-1)}|\kappa, m-1\rangle \tag{24b}$$

$$\hat{K}_0|\kappa, m\rangle = m|\kappa, m\rangle \tag{24c}$$

where m can take the values

$$m = \kappa, \kappa+1, \ldots \tag{25}$$

for the Bargmann index κ which characterizes the irreducible representation.

Since the generators (20*a*), (20*b*) and (20*c*) satisfy the $su(1,1)$ algebra, we need to establish the connection between $\{\kappa, m\}$ and the quantum numbers $\{\sigma, n\}$ in order to recover (24). This goal is accomplished by comparing the eigenvalues of the K_0 operator. It is straightforward to obtain that $\kappa = \sigma$ and $m = \sigma + n$. Since n can take any positive integer value $n = 0, 1, \ldots,$ we have

$$m = \sigma, \sigma+1, \ldots \tag{26}$$

in accordance with (25). Finally, the Casimir operator can be written as

$$\hat{C} = \hat{K}_+\hat{K}_- - \hat{K}_0(\hat{K}_0 - 1) = \hat{K}_-\hat{K}_+ - \hat{K}_0(\hat{K}_0 + 1) \tag{27}$$

with eigenvalues

$$\hat{C}\Phi_n^\sigma(y) = -\sigma(\sigma-1)\Phi_n^\sigma(y) \tag{28}$$

as expected.

Although the operators $\hat{K}_\pm$ are not symmetrical, the unitary representation, equation (24), assures that $\hat{K}_\pm = \hat{K}_\mp^\dagger$ through the matrix elements

$$\langle\Psi_{n\pm1}|\hat{K}_\pm|\Psi_n\rangle = \left\langle\hat{K}_\pm^\dagger\Psi_{n\pm1}\middle|\Psi_n\right\rangle = \langle\hat{K}_\mp\Psi_{n\pm1}|\Psi_n\rangle. \tag{29}$$

We have thus established the algebra associated with the basis (15). These functions are not eigenfunctions of the Morse Hamiltonian, but it is possible to express the Hamiltonian, as well as any dynamical variable, in terms of the algebra

$$G_{su(1,1)} = \{\hat{K}_+, \hat{K}_-, \hat{K}_0\}. \tag{30}$$

Consequently, the $su(1,1)$ algebra can be considered as a suitable dynamical algebra for the Morse system in the space $\mathcal{L}_\sigma$. In this algebraic space, the basis (15) takes the simple form

$$\left|\Phi_n^\sigma\right\rangle = G_n^\sigma(\hat{K}_+)^n\left|\Phi_0^\sigma\right\rangle \tag{31}$$

where the normalization constant is given by

$$G_n^\sigma = \sqrt{\frac{\Gamma(2\sigma)}{n!\Gamma(2\sigma+n)}}. \tag{32}$$

We now proceed to establish the Hamiltonian in the algebraic space (30).

3. Hamiltonian

In this section we shall write the Hamiltonian in the $su(1,1)$ space. In order to express the Morse Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + D(\mathrm{e}^{-2\beta x} - 2\,\mathrm{e}^{-\beta x}) \tag{33}$$

in terms of the $su(1, 1)$ algebra, we first note that the potential (1) can be rewritten as

$$V(y) = \frac{D}{(2j+1)}\left(\frac{y^2}{(2j+1)} - 2y\right) \tag{34}$$

and that the coordinate y and the momentum $\hat{p} = -\mathrm{i}\hbar\,\mathrm{d}/\mathrm{d}x = i\hbar\beta y\,\mathrm{d}/\mathrm{d}y$ are related to $\hat{K}_\pm$ (20a), (20b) by

$$\hat{p} = \frac{\mathrm{i}\hbar\beta}{2}(\hat{K}_+ - \hat{K}_-) \tag{35a}$$

$$y = 2\hat{K}_0 - (\hat{K}_+ + \hat{K}_-). \tag{35b}$$

Substituting (35) into (33), we obtain the Hamiltonian

$$\hat{H} = \frac{\hbar^2\beta^2}{2\mu}\left\{-\sigma(\sigma-1) + \hat{K}_0(2\hat{K}_0 - 2j - 1) + (j + 1/2)(\hat{K}_+ + \hat{K}_-) - \tfrac{1}{2}[(\hat{K}_+ + \hat{K}_-)\hat{K}_0 + \hat{K}_0(\hat{K}_+ + \hat{K}_-)]\right\} \tag{36}$$

where we have taken into account that

$$D = \frac{\hbar^2\beta^2}{8\mu}(2j+1)^2. \tag{37}$$

The only non-null matrix elements of $\hat{H}$ in the basis (15) are given by

$$\left\langle \Phi_n^\sigma \middle| \hat{H} \middle| \Phi_n^\sigma \right\rangle = \frac{\hbar^2\beta^2}{2\mu}[-\sigma(\sigma-1) + (\sigma+n)(2\sigma+2n-2j-1)] \tag{38a}$$

$$\left\langle \Phi_{n+1}^\sigma \middle| \hat{H} \middle| \Phi_n^\sigma \right\rangle = \frac{\hbar^2\beta^2}{2\mu}[(j-\sigma-n)\sqrt{(n+1)(2\sigma+n)}] \tag{38b}$$

$$\left\langle \Phi_{n-1}^\sigma \middle| \hat{H} \middle| \Phi_n^\sigma \right\rangle = \frac{\hbar^2\beta^2}{2\mu}[(j-\sigma-n+1)\sqrt{n(2\sigma+n-1)}]. \tag{38c}$$

A remarkable property of this representation is that it is possible to choose the parameter σ in such a way that the non-diagonal contributions vanish for a given n. Imposing this condition on (38b), we have $j - \sigma - n = 0$, which means that

$$n = j - \sigma. \tag{39}$$

We thus have that fixing the parameter σ we select n at which the Hamiltonian matrix splits into two blocks. In particular, for $\sigma = j - [j]$ the first block corresponds to $[j] + 1$ functions and establishes a complete basis for the bound states.

As an example, for the case of a Morse potential with $j = 4$ and a basis generated with $\sigma = 1$, in figure 2 we show the states obtained as the number of basis states increases from 4 to 20. As we can see the states are densely packed near the dissociation threshold, while their density diminishes as the energy increases. The inset is a zoom of the low energy part. Energies are given in units of $\hbar^2\beta^2/\mu$. It can be seen that, for this selection of σ with four states in the basis, the bound states are reproduced exactly.

By choosing $\sigma = j - [j]$ it is possible to distinguish between the bound and continuum parts of the spectrum. From the group theoretical point of view the $su(1, 1)$ representation corresponding to $\sigma = j - [j]$ provides a subspace carrying the $su(2)$ irreps characterized by j. Note that the block diagonal form of the Hamiltonian matrix implies the following orthogonal relation between the basis states $\Phi_n^{j-[j]}$ (15) and the exact Morse bound states Ψ_v^j (2):

$$\left\langle \Phi_n^{j-[j]} \middle| \Psi_v^j \right\rangle = 0 \qquad n \geqslant [j] + 1. \tag{40}$$

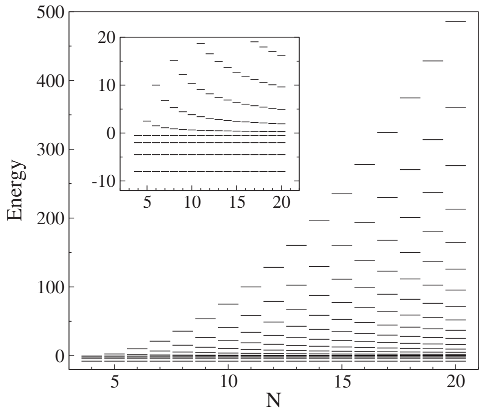

Figure 2. Energy eigenvalues (dimensionless, in units of $\hbar^2\beta^2/\mu$), for the Morse potential with $j = 4$ as a function of the size of the basis N generated for $\sigma = 1$. The inset is a zoom of the low energy region.

This result can be obtained by the explicit calculation of the matrix elements but we present now the reason for that. A Morse potential characterized by j has $[j] + 1$ bound states which are the only normalizable eigenstates of the Morse Hamiltonian in the complete Hilbert space. If we take $\sigma = j - [j]$, we get that in our basis, equation (15), the states characterized by $n = 0, 1, \ldots, [j]$ decouple from the rest. Consequently, the eigenstates of the Hamiltonian in this basis should be eigenstates of the Hamiltonian in the complete space too. Hence, the basis functions with $n > [j]$, which obviously are orthogonal to the basis states with $n \leqslant [j]$, must also be orthogonal to the actual bound states of the Morse Hamiltonian as stated in (40).

4. Interpretation of the basis $\Phi_n^\sigma(y)$

In order to interpret the family of orthonormal functions (15) we shall introduce rising and lowering operators of the Morse bound functions (2) which shift the number of quanta, as well as the potential parameter j.

Applying the operator $y\frac{\mathrm{d}}{\mathrm{d}y}$ to (2), we have

$$y\frac{\mathrm{d}}{\mathrm{d}y}\Psi_v^j(y) = \left[-\tfrac{1}{2}y + (j-v)\right]\Psi_v^j(y) + N_v^j y^{j-v} y\,\mathrm{e}^{-y/2}\frac{\mathrm{d}}{\mathrm{d}y}L_v^{2(j-v)}(y). \tag{41}$$

If we introduce relation (18), the following equation is obtained:

$$\Psi_{v-1}^{j-1}(y) = N_{v-1}^{j-1}\,\mathrm{e}^{-y/2} y^{j-v} L_{v-1}^{2j-2v}(y). \tag{42}$$

We can introduce the operators

$$\hat{A}_\pm(q) = \pm y\frac{\mathrm{d}}{\mathrm{d}y} - \frac{1}{2}y + q \tag{43}$$

where q is a parameter. It is straightforward to obtain the action of this type of operators on the bound states for the Morse Hamiltonian, equation (2),

$$\hat{A}_-(j)\Psi_v^j(y) = m_-\Psi_{v-1}^{j-1}(y) \qquad \text{with} \quad m_- = \sqrt{v(2j-v)} \tag{44}$$

$$\hat{A}_+(j+1)\Psi_v^j(y) = m_+\Psi_{v+1}^{j+1}(y) \qquad \text{with} \quad m_+ = \sqrt{(v+1)(2j-v+1)}. \tag{45}$$

From the definition of the $\hat{A}$ operators it is clear that

$$[\hat{A}_+(q), \hat{A}_+(q')] = 0. \tag{46}$$

The operators $\hat{A}_\pm$ correspond essentially to the operators $\hat{T}_\pm$ given by Cooper *et al* [44], which are related to the potential group approach for the Morse potential [45, 46]. The reason why the operators (43) turn out to be similar to the operators associated with the Morse eigenfunctions will become clear at the end of the section.

Now we can obtain the action of the new operators $\hat{A}_\pm(q)$ on our basis functions, equation (15), using equations (21*a*) and (21*b*):

$$\hat{A}_+(\sigma + n)\Phi_n^\sigma(y) = k_+\Phi_{n+1}^\sigma(y) \tag{47}$$

$$\hat{A}_-(\sigma + n)\Phi_n^\sigma(y) = k_-\Phi_{n-1}^\sigma(y). \tag{48}$$

Thus the action of the new operators $\hat{A}_\pm(q)$ on the basis wavefunctions and on the Morse bound states is known.

Let us come back to the selection rule (40), but now from the point of view of the new operators (43). From the definition of $\hat{A}_+(q)$ we can write the Morse wavefunctions in terms of successive application of appropriate $\hat{A}_+$ operators over $\Psi_0^{j-v}(y)$,

$$\left|\Psi_v^j\right\rangle = B_v^j \prod_{\alpha=1}^{v} \hat{A}_+(j - v + \alpha)\left|\Psi_0^{j-v}\right\rangle \tag{49}$$

where

$$B_v^j = \sqrt{\frac{(2j - 2v)!}{v!(2j - v)!}}. \tag{50}$$

From the expression of the Morse bound states, equation (2), and the definition of the basis states in equation (15) the following equation is obtained:

$$\Psi_0^{j-v}(y) = \frac{N_0^{j-v}}{A_0^\sigma} y^{j-v-\sigma}\Phi_0^\sigma(y). \tag{51}$$

From the definition of the $\hat{A}_\pm$ operators the expression of y as a function of them can be written as

$$y = q + q' - (\hat{A}_+(q) + \hat{A}_-(q')). \tag{52}$$

With equations (49)–(52) the Morse bound states can be expressed as

$$\left|\Psi_v^j\right\rangle = B_v^j \frac{N_0^{j-v}}{A_0^\sigma} \prod_{\alpha=1}^{v} \hat{A}_+(j - v + \alpha)[q + q' - (\hat{A}_+(q) + \hat{A}_-(q'))]^{j-v-\sigma}\left|\Phi_0^\sigma\right\rangle. \tag{53}$$

Then the overlap between a basis state and a Morse bound state wavefunction is

$$\left\langle\Phi_n^\sigma\middle|\Psi_v^j\right\rangle = G_n^\sigma B_v^j \frac{N_0^{j-v}}{A_0^\sigma}\left\langle\Phi_n^\sigma\right| \prod_{\alpha=1}^{v} \hat{A}_+(j - v + \alpha)[q + q' - (\hat{A}_+(q) + \hat{A}_-(q'))]^{j-v-\sigma}\left|\Phi_0^\sigma\right\rangle. \tag{54}$$

The action of the operators $\hat{A}_+$ and $\hat{A}_-$ on $\left|\Phi_0^\sigma\right\rangle$ generates a linear combination of functions $\left|\Phi_\zeta^\sigma\right\rangle$, with $\zeta = 0, 1, 2, \ldots, j - \sigma$, as established by (47) and (48). Consequently, the overlap $\left\langle\Phi_n^\sigma\middle|\Psi_v^j\right\rangle$ reduces to a linear combination of products $\left\langle\Phi_n^\sigma\middle|\Phi_\zeta^\sigma\right\rangle$, all of which vanish as long as $n > j - \sigma$. This result, together with the selection $\sigma = j - [j]$, leads to the orthogonality condition (40) previously obtained in coordinate space.

The operators $\hat{A}_\pm$ can help us in establishing a relation between our basis states and the Morse wavefunctions. In the same way as in equation (49), from the definition for $\hat{A}_+(q)$

given above we can write the basis wavefunctions $\Phi_n^\sigma(y)$ in terms of successive applications of $\hat{A}_+$ over $\Phi_0^\sigma(y)$

$$\left|\Phi_n^\sigma\right\rangle = G_n^\sigma \prod_{\beta=1}^{n} \hat{A}_+(\sigma - 1 + \beta)\left|\Phi_0^\sigma\right\rangle \tag{55}$$

with the normalization given by (32). Noting that $\left|\Psi_0^\sigma\right\rangle = \left|\Phi_0^\sigma\right\rangle$ we can write equation (55) as

$$\left|\Phi_n^\sigma\right\rangle = G_n^\sigma \hat{A}_+(\sigma) \prod_{\beta=2}^{n} \hat{A}_+(\sigma - 1 + \beta)\left|\Psi_0^\sigma\right\rangle. \tag{56}$$

If we now identify the function $\left|\Psi_{n-1}^{\sigma+n-1}\right\rangle$ according to (45), we have

$$\left|\Phi_n^\sigma\right\rangle = \sqrt{\frac{1}{(2\sigma)n}}\hat{A}_+(\sigma)\left|\Psi_{n-1}^{\sigma+n-1}\right\rangle. \tag{57}$$

If we now take into account that

$$\hat{A}_+(\sigma) = \hat{A}_+(\sigma + n) - n \tag{58}$$

we arrive at the result

$$\left|\Phi_n^\sigma\right\rangle = \sqrt{\frac{(2\sigma + n)}{2\sigma}}\left|\Psi_n^{\sigma+n}\right\rangle - \sqrt{\frac{n}{2\sigma}}\left|\Psi_{n-1}^{\sigma+n-1}\right\rangle. \tag{59}$$

The family of functions $\Phi_n^\sigma(y)$ is then a linear combination of Morse-like functions with potential parameters $\sigma + n$ and $\sigma + n - 1$. This result explains the resemblance of the operators (43) to the operators obtained in the potential approach. The functions (15) turn out to be Morse-like functions associated with different potential depths.

Finally, we should note that the Morse Hamiltonian can be factorized in the form

$$\hat{H} = \frac{\hbar^2\beta^2}{2m}\hat{A}_+(j)\hat{A}_-(j) - \hbar\omega j^2 \tag{60}$$

the expression for which is derived from supersymmetric quantum mechanics [47]. The matrix elements of this operator in the basis $\left|\Phi_n^\sigma\right\rangle$ are obtained by means of the transformations

$$\hat{A}_\pm(j) = \hat{A}_\pm(\sigma + n) + (j - \sigma - n) \tag{61}$$

which when applied to (60), lead to the matrix elements (38). The connection of the operators $\hat{A}_\pm$ with the factorization (60) is a consequence of the relation between the factorization method and the concept of shape-invariant potentials discussed in supersymmetric quantum mechanics [48].

5. Dipole function

Once the Hamiltonian has been diagonalized we obtain the energy spectrum as well as the eigenfunctions. In general, a good description of the energy spectrum is not necessarily accompanied by high quality of the eigenstates. It is thus necessary to check the eigenfunctions through the evaluation of relevant observables. One of the most important observables is the dipole transition operator. We shall thus present here the matrix elements of the dipole operator.

In general the form of the bond dipole function is not known. One possibility is to express the dipole function as a Taylor series expansion around the equilibrium positions in terms of a function of the instantaneous bond lengths. For instance, in terms of the variable $z = 1 - \mathrm{e}^{-\beta x}$:

$$\mu(x) = \sum_{p=0}^{P} \frac{z^p}{p!}\left(\frac{\mathrm{d}^p\mu}{\mathrm{d}z^p}\right)_e \tag{62}$$

where we have considered a finite sum. An alternative choice is the use of an analytical function such as the commonly used Mecke dipole operator function [49, 50]

$$\hat{\mu}(x) = d_0 x^{\xi}\, e^{-\gamma x} \tag{63}$$

where d_0 and γ are adjustable parameters. Often ξ is taken to be an integer $\geqslant 1$. We thus intend to obtain the matrix elements of (63) in the basis (15)

$$\mu_{mn} = \left\langle \Phi_m^\sigma \middle| \hat{\mu}(x) \middle| \Phi_n^\sigma \right\rangle. \tag{64}$$

We shall not proceed directly with the calculation. Instead we first note that

$$\mu_{mn} = d_0(-1)^{\xi} \frac{\partial^{\xi}}{\partial \gamma^{\xi}} \left\langle \Phi_m^\sigma \middle| \hat{T} \middle| \Phi_n^\sigma \right\rangle \tag{65}$$

where

$$\hat{T} = e^{-\gamma x}. \tag{66}$$

We shall thus pay attention to the calculation of the matrix elements of the latter operator, and later on recover the required matrix elements μ_{nm} through (65).

In the $su(1,1)$ space the matrix elements are given by

$$\left\langle \Phi_m^\sigma \middle| \hat{T} \middle| \Phi_n^\sigma \right\rangle = G_m^\sigma G_n^\sigma \left\langle \Phi_0^\sigma \right| \prod_{\beta=1}^{m} \hat{A}_-(\sigma - 1 + \beta) \hat{T} \prod_{\beta'=1}^{n} \hat{A}_+(\sigma - 1 + \beta') \left| \Phi_0^\sigma \right\rangle. \tag{67}$$

Here we shall consider the case $m \leqslant n$ only, since the matrix is symmetric. In order to compute these matrix elements we first obtain the commutators

$$[\hat{A}_-(q), \hat{T}] = \left[\frac{1}{\beta}\frac{d}{dx}, \hat{T}\right] = -\frac{\gamma}{\beta}\hat{T} \tag{68a}$$

$$[\hat{A}_+(q), \hat{T}] = \left[-\frac{1}{\beta}\frac{d}{dx}, \hat{T}\right] = \frac{\gamma}{\beta}\hat{T}. \tag{68b}$$

To compute (67) we use the relation

$$\hat{A}_-(n) = \hat{A}_-(m) + (n - m). \tag{69}$$

There is a similar expression for the rising operator. Taking into account (68) and (69), we obtain the following result,

$$\left\langle \Phi_m^\sigma \middle| \hat{T} \middle| \Phi_n^\sigma \right\rangle = f_1(\sigma, m, n) \sum_{\zeta=0}^{m} f_2(\sigma, m, n, \zeta) g(\sigma, j, m, n, \zeta; \alpha) \tag{70}$$

where we have defined $\alpha = \gamma/\beta$, and the functions are given by

$$f_1(\sigma, m, n) = \sqrt{\frac{m!n!\Gamma(2\sigma + n)}{\Gamma(2\sigma + m)}} \tag{71a}$$

$$f_2(\sigma, m, n, \zeta) = \frac{1}{\zeta!(m-\zeta)!(n-\zeta)!\Gamma(2\sigma + n - \zeta)} \tag{71b}$$

and

$$g(\sigma, j, m, n, \zeta; \alpha) = \frac{\Gamma(2\sigma + \alpha)}{(2j+1)^{\alpha}} (-\alpha - n - \zeta)_{m-\zeta} (-\alpha)_{n-\zeta} \tag{72}$$

where $(a)_n$ stands for a Pochhammer symbol. The dipole matrix elements are obtained by (65)

$$\mu_{mn} = (-1)^{\xi} \frac{d_0}{\beta^{\xi}} f_1(\sigma, m, n) \sum_{\zeta=0}^{m} f_2(\sigma, m, n, \zeta) \frac{\partial^{\xi}}{\partial \alpha^{\xi}} g(\sigma, j, m, n, \zeta; \alpha) \tag{73}$$

where we have taken into account the chain rule

$$\frac{\partial}{\partial \gamma} = \frac{1}{\beta} \frac{\partial}{\partial \alpha}. \tag{74}$$

In particular, for the case $\xi = 1$, the first derivative is needed

$$\begin{aligned} \frac{\partial g(\sigma, j, m, n, \zeta; \alpha)}{\partial \alpha} &= g(\sigma, j, m, n, \zeta; \alpha)\{\ln(2j+1) + \psi(m-n-\alpha) - \psi(-\alpha) \\ &\quad + \psi(n-\alpha-\zeta) - \psi(-n-\alpha+\zeta) - \psi(2\sigma+\alpha)\} \end{aligned} \tag{75}$$

where $\psi(n)$ is the digamma function. It is worth noting that this expression can give numerical problems if α is an integer. In that case, one can make directly the derivative of equation (72) using the following definition of the derivative of a Pochhammer symbol valid when a is a negative integer:

$$\frac{\mathrm{d}(a)_n}{\mathrm{d}a} = \begin{cases} (a)_n \sum_{i=0}^{n-1} \frac{1}{a+i} & \text{if} \quad n \leqslant -a \\ (-1)^a (-a)!(n+a-1)! & \text{if} \quad n > -a. \end{cases}$$

Let us come back to the dipole moment in terms of the expansion (62). If we were interested in the first terms of the expansion only, we could directly use equation (35*b*):

$$z = \left(1 - \frac{y}{2j+1}\right) = 1 - \frac{1}{2j+1}[2K_0 - K_+ - K_-]. \tag{76}$$

However, a closed expression for any power of z can be obtained in terms of the matrix elements (70). Since

$$z^p = (1 - \mathrm{e}^{-\beta x})^p = \sum_{q=0}^{p} \frac{p!}{q!(p-q)!} (-1)^{p-q} \, \mathrm{e}^{-\beta(p-q)x} \tag{77}$$

we have

$$\left\langle \Phi_m^{\sigma} \middle| z^p \middle| \Phi_n^{\sigma} \right\rangle = \sum_{q=0}^{p} \frac{p!}{q!(p-q)!} (-1)^{p-q} \left\langle \Phi_m^{\sigma} \middle| \hat{T} \middle| \Phi_n^{\sigma} \right\rangle \tag{78}$$

where in this case $\alpha = p - q$. We have thus provided closed expressions for both forms (62) and (63) of the dipole functions. The matrix elements for the generalization of (63) to $\xi > 1$ can in principle be obtained by taking multiple derivatives of (70).

As an illustration of the results that can be obtained, we have performed a simple calculation with the Mecke dipole operator function

$$\hat{\mu}(x) = x \, \mathrm{e}^{-x}. \tag{79}$$

We use dimensionless variables in such a way that energies are given in units of $\hbar^2\beta^2/\mu$ and distances are given in units of β^{-1}. We consider a Morse potential with $j = 4$ and calculate from the bound states the transition strength (S) and the energy weighted transition strength (E_W) defined as $S(\hat{\mu}; n, m; N) = |\langle N, m|\hat{\mu}|N, n\rangle|^2$ and $E_W(\hat{\mu}; n, m; N) = \left(e_n^N - e_m^N\right)|\langle N, m|\hat{\mu}|N, n\rangle|^2$, where e_n^N is the energy of the state n in a basis of N functions. In figure 3 we present the strengths for a calculation with a basis with $N = 20$ states. The left panels give transition strengths starting from different initial states: in the upper

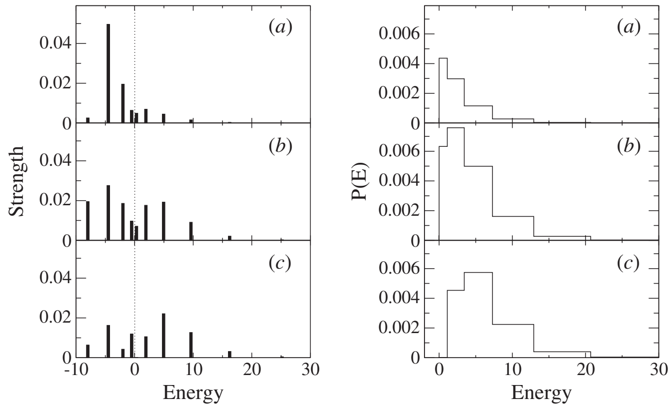

Figure 3. Transition strength to all states (left panels) and probability density for transitions to the continuum (right panels) from the ground state (*a*), from an average with equal weights of all bound states (*b*) and from the least bound state (*c*). The diagonal terms are also included. The dipole operator used is given in equation (79). The calculation is done with a basis generated for $\sigma = 1$ of $N = 20$ states for a Morse potential with $j = 4$. The probability density to the continuum is represented as an histogram as explained in the text.

Table 1. Convergence of the total strength (*S*) and energy weighted sum rule (E_W) to the continuum for the operator $\hat{\mu} = x\,\mathrm{e}^{-x}$ as a function of the discrete basis dimension generated for $\sigma = 1$ for the Morse Hamiltonian with $j = 4$. Two cases are presented: one with the ground state as the initial state and the other with the least bound state as the initial state. *N* is the total number of basis states.

	$n = 0$		$n = 3$	
N	$S(\hat{\mu}, N)$	$E_W(\hat{\mu}, N)$	$S(\hat{\mu}, N)$	$E_W(\hat{\mu}, N)$
6	0.018 1201	0.203 022	0.046 1536	0.397 858
8	0.018 1261	0.202 675	0.048 5419	0.342 468
10		0.202 672	0.048 7340	0.338 792
20			0.048 7918	0.337 513
30			0.048 7931	0.337 464
Exact value	0.018 1261	0.202 672	0.048 7933	0.337 450

panel the initial state is the ground state ($n = 0$), in the middle panel the initial state is an average with the same weight of all bound states and in the lower panel the initial state is the least bound state ($n = 3$). The diagonal strengths are also included. The right panels give the corresponding probability densities for transitions to the continuum. Since our basis is discrete we have distributed the strength to each state E_i in the continuum in an energy interval $\Delta E_i = [(E_i + E_{i-1})/2, (E_i + E_{i+1})/2]$ and represent it as an histogram. It can be seen that the maximum of the distribution moves up in energy as the initial state is less bound and the total strength to the continuum is larger also when the initial state is less tightly bound. In table 1 we investigate the convergence of the total strength and the energy weighted sum rule from the initial state n to the continuum as a function of the number of basis states included. Both of these magnitudes can be calculated exactly and, in our case, are $S(\hat{\mu}; n, N) = \sum_{i=4}^{N-1} S(\hat{\mu}; n, i; N)$ and $E_W(\hat{\mu}; n; N) = \sum_{i=4}^{N-1} E_W(\hat{\mu}; n, i; N)$, respectively. In table 1 we present the results for two different initial states: the ground state ($n = 0$) and the least bound state ($n = 3$). Table 1 shows that for the case starting in the ground state the convergence is fast and with $N = 10$ the exact values for both total strength and energy weighted sum rule are obtained. For the least favourable case starting in $n = 3$ a basis of $N = 10$ states (six states in the continuum) provides a good approximation to the exact values (errors are of the order of 1 per thousand). It is worth noting that in figure 3(*c*) the transition operator used populates very weakly (it is not seen on the scale used) the lowest energy state in the continuum. This clearly deviates from the harmonic image and shows the anharmonic nature of the potential.

6. Summary and conclusions

In this paper we propose an $su(1,1)$ dynamical algebra to describe both the discrete and the continuum parts of the spectrum for the Morse potential. The basic idea consists in considering the orthonormal polynomials with respect to the weighting function $w(y) = \mathrm{e}^{-y} y^{2\sigma-1}$, which define a family of possible bases to describe the complete spectrum of the system. In terms of these bases the matrix representation of the Hamiltonian is tridiagonal, which is an advantage when considering large bases. The raising and lowering operators associated with this family of polynomials satisfy the $su(1,1)$ commutation relations. Particularly important is the case of $\sigma = j - [j]$ (j is related to the depth of the Morse potential considered and $[j]$ is the closest integer to j that is smaller than j) for which the discrete and continuum parts of the spectrum are decoupled. The orthogonality relation (40) associated with this property is proved in both configuration and algebraic representations. We have also shown that the functions (15) correspond to Morse-like functions associated with different potential depths. This identification establishes the connection with previous analysis in terms of supersymmetric quantum mechanics. In addition, an analytical expression for the Mecke dipole moment function has been obtained. A general Taylor expansion of the dipole function is also discussed.

In the algebraic approach the Hamiltonian as well as any dynamical variable can be expanded in terms of the $su(1,1)$ generators. In particular, the momentum and the Morse coordinate y turn out to be linear in the generators. This fact has important consequences when dealing with realistic systems. The interactions of a molecular Hamiltonian can be represented in exact form in the $su(1,1)$ space. This result is in contrast to the description of the Morse bound states in the $su(2)$ space (10). In such a case the momenta and coordinates are expanded in terms of a series in terms of powers of the parameter $1/\sqrt{2j+1}$, which can be cut reasonably up to order $1/\sqrt{2j+1}$, although in most applications only linear terms are considered.

The linear representation of the coordinates and momenta in the generators of the $su(1,1)$ algebra explains why the matrix representation of the Hamiltonian is tridiagonal. This result, together with the fact that the matrix elements of the Hamiltonian have been obtained in closed form, allows us to carry out calculations of realistic systems. In general, one of the advantages of the algebraic approach consists in obtaining matrix elements in analytic form. In this vein we have obtained a closed expression for the matrix elements of the Hamiltonian as well as for the Mecke dipole function, which becomes important in the calculation of dipole transition intensities.

In comparison with the description of the bound states in terms of the $su(2)$ algebra, the $su(1,1)$ framework has the advantage previously mentioned of considering in exact form the expansion of the coordinates and momenta, although the dimension of the space may increase considerably in order to take into account the continuum. We believe, however, that in the framework of the $su(1,1)$ scheme it will be possible to deal with molecular systems near the dissociation limit or even to study the dissociation process itself.

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