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2004 J. Phys. A: Math. Gen. 37 877

(http://iopscience.iop.org/0305-4470/37/3/023)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **37** (2004) 877–893 PII: S0305-4470(04)67667-0

An *su*(1, 1) dynamical algebra for the Pöschl–Teller potential

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Received 11 August 2003
Published 7 January 2004
Online at stacks.iop.org/JPhysA/37/877 (DOI: 10.1088/0305-4470/37/3/023)

Abstract

An $su(1, 1)$ dynamical algebra to describe the continuum part of the spectrum for the modified Pöschl–Teller 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 corresponding to a Pöschl–Teller ground state. An analysis of the associated algebra is investigated in detail. The functions are identified with Pöschl–Teller-like functions associated with different potential depths. We prove that by choosing appropriately the parameter σ it is possible to decouple the discrete states of a given parity from the continuum part of the spectrum. A discussion of the matrix elements of the dipole function operator is also included.

PACS number: 03.65.−w

1. Introduction

The study of quantum systems from the point of view of symmetry has attracted attention since the early days of quantum mechanics [1]. The family of solvable potentials is particularly important since detailed analytical studies are possible [2]. Among the solvable systems, the Pöschl–Teller (PT) potential [3, 4] has been widely analysed from different perspectives [5–15]. This potential presents bound and scattering states, and both regions of the spectrum have been studied. The PT potential, together with the Morse potential, represent the most studied anharmonic potentials, both of them having in common their relation with the $SO(2, 1)$ and $SU(2)$ groups [16]. The associated $su(2)$ algebra constitutes a dynamical algebra for the discrete part of the spectrum, which means that any variable can be expanded in terms of the generators of the $su(2)$ algebra, as long as we deal with the bound region of the spectrum [16]. The $so(2, 1)$ algebra, on the other hand, arises in scattering states [6] as well as in the potential group approach, where wavefunctions associated with different potentials, but the

same energy, are connected. Closely related with the Schrödinger method of factorization [17, 18] is the supersymmetry approach, whose generalized operator method quickly yields all the bound state energy eigenvalues, eigenfunctions as well as the scattering matrix [5]. Recently, in the framework of supersymmetric quantum mechanics extended to deal with non-Hermitian Hamiltonians, a related PT complex potential with real spectra was derived by a potential algebraic approach based upon the complex Lie algebra $sl(2, C)$ [9–11]. Both algebras $so(2, 1)$ and $sl(2, C)$, as well as $su(1, 1)$, are isomorphic. In this work we shall introduce the $su(1, 1)$ algebra as the dynamical algebra of the PT potential associated with both the discrete and continuum spectra.

The PT potential has been proved to be a suitable potential to deal with the out-of-plane bending vibrations [19]. In a local mode description for molecular vibrational excitations an anharmonic potential is associated with each internal degree of freedom [20–23]. A Morse potential is associated for the stretches, while for the bendings harmonic potentials are usually proposed, although either a Morse or PT potential may be used, depending of the symmetry of the potential [24]. The potential associated with the out-of-plane local coordinate is symmetric, a feature that suggests using a PT potential for its description. Although the Morse and PT potentials are similar concerning the dynamical symmetry, from the technical point of view they are quite different. While for the Morse potential closed analytic results for different matrix elements have been obtained, more involved expressions are given for the PT potential. In both cases, however, only the discrete part of the spectra is considered, neglecting the continuum part of the space. For excitations in the high energy region of the spectrum near the chemical threshold, a complete basis becomes compulsory, since eventually the dissociation may take place.

Due to its importance, great attention has been paid to incorporate the continuum, appropriately discretized, in the description of quantum mechanical systems [25–31]. Recently, the use of a transformed harmonic oscillator (THO) basis has been proposed to describe the effect of the continuum by means of a discrete basis, which is determined by the ground state of the system [32]. In this work we present an alternative to the THO basis to establish a complete basis for the PT oscillator to describe both the discrete and the continuum parts of the spectrum for the PT potential. We prove that an $su(1, 1)$ algebra is the dynamical algebra associated with the complete space and show that the functions of this basis correspond to PT-like functions associated with different potential depths, a fact that establishes a link with the potential approach.

In section 2 we present a summary of the bound state solutions for the PT potential, making explicit the connection with the $su(2)$ algebra. Section 3 is devoted to presenting the complete basis set as well as the proof that its ladder operators constitute an $su(1, 1)$ dynamical algebra for the system. The matrix elements of the Hamiltonian are obtained in section 4. In section 5 we present an algebraic interpretation of the basis, and discuss the relation with supersymmetry. In section 6 we present model calculations for an operator which couples the bound state to the continuum, as well as a discussion concerning the calculation of the dipole moment matrix elements. Finally, in section 7 a summary and our conclusions are presented.

2. Bound eigenfunctions for the Pöschl–Teller potential

We start by reviewing the analytic and algebraic treatment of the bound solutions for the modified Pöschl–Teller potential (MPT), which is given by [3]

$$V(x) = -\frac{D}{\cosh^2(\alpha x)} \tag{1}$$

where $D > 0$ corresponds to its depth, α is related to the range of the potential, and x is the physical displacement variable which may correspond to the internal coordinate considered to describe a molecular bending mode.

The solution of the Schrödinger equation associated with the potential (1) is given by [33, 34]

$$\Psi_v^j(u) = N_v^j (1-u^2)^{\frac{j-v}{2}} C_v^{j+1/2-v}(u) \tag{2}$$

where $C_v^\lambda(u)$ are the Gegenbauer polynomials and the normalization constant is given by

$$N_v^j = \sqrt{\frac{\alpha v! \Gamma[j-v+1/2]}{\pi^{1/2}\Gamma[j-v]\,(2j-2v+1)_v}} \tag{3}$$

where $(a)_n$ stands for a Pochhammer symbol [35]. The argument u is related with the physical displacement coordinate x by $u = \tanh(\alpha x)$. The index j is connected with the potential depth through

$$j(j+1) = \frac{2\mu D}{\alpha^2 \hbar^2}. \tag{4}$$

The number of quanta v takes the values $0, 1, 2, \ldots, v_{\max}$ and, together with j, gives the energy

$$j - v = \sqrt{\frac{-2\mu E}{\alpha^2 \hbar^2}} \tag{5}$$

where μ is the reduced mass of the molecule. The corresponding energy spectrum is

$$E_v = -\hbar\omega(j-v)^2 = -\frac{\hbar^2\alpha^2}{2\mu}(j-v)^2. \tag{6}$$

From the dissociation condition in (6)

$$j - v \geqslant 0 \tag{7}$$

and consequently the expected maximum number of quanta is

$$v_{\max} = [j] \tag{8}$$

where $[j]$ stands for the closest integer to j that is smaller than j.

It is possible to obtain an algebraic representation of the solutions (2) by introducing creation $\hat{b}^\dagger$ and annihilation $\hat{b}$ operators [14], which have the following action on the functions (2)

$$\hat{b}^\dagger \Psi_v^j(u) = \sqrt{(v+1)(1-(v+1)/(2j+1))}\,\Psi_{v+1}^j(u) \tag{9a}$$

$$\hat{b}\Psi_v^j(u) = \sqrt{v(1-v/(2j+1))}\,\Psi_{v-1}^j(u) \tag{9b}$$

with the following definition

$$\hat{v}\Psi_v^j(u) = v\Psi_v^j(u). \tag{10}$$

It is clear that the operator $\hat{v}$ is well defined as long as the action is given over the eigenfunction space $\Psi_v^j(u)$. The operators $\{b^\dagger, b\}$, together with the number operator $\hat{v}$, satisfy the commutation relations

$$[\hat{b}, \hat{b}^\dagger] = 1 - \frac{2\hat{v}+1}{(2j+1)} \qquad [\hat{v}, \hat{b}^\dagger] = \hat{b}^\dagger \qquad [\hat{v}, \hat{b}] = -\hat{b} \tag{11}$$

which can be identified with the usual $su(2)$ commutation relations by introducing the set of transformations $\left\{b^\dagger = \hat{J}_-/\sqrt{(2j+1)}, b = \hat{J}_+/\sqrt{(2j+1)}, \hat{v} = j - \hat{J}_0\right\}$, where J_μ satisfy the

usual 'angular momentum' commutation relations [36]. The projection m is related with v by [37]

$$m = v - j. \tag{12}$$

From this relation we see that the ground state ($v = 0$) corresponds to $m = -j$. The MPT functions (2) are then associated with one branch (in this case to $m < 0$) of the $su(2)$ representations. The $su(2)$ group is the dynamical symmetry for the bound states for the MPT potential and any dynamical variable can be expanded in terms of the generators

$$G_{su(2)} = \{\hat{b}^\dagger, \hat{b}, \hat{v}\}. \tag{13}$$

For a MPT potential with $[j] + 1$ bound states, the functions (2) acquire in the algebraic space the simple form

$$\left|\Psi_v^j\right\rangle = \mathcal{N}_v^j (\hat{b}^\dagger)^v \left|\Psi_0^j\right\rangle \tag{14}$$

with normalization constant

$$\mathcal{N}_v^j = \sqrt{\frac{(2j+1)^v}{v!(2j-v+1)_v}}. \tag{15}$$

In the $su(2)$ space the variable u, as well as 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 [15].

3. An orthonormal complete basis for the Pöschl–Teller potential

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,

$$\Phi_n^\sigma(u) = A_n^\sigma (1-u^2)^{\frac{\sigma}{2}} C_n^{\sigma-1/2}(u) \qquad n = 0, 1, 2, \ldots \tag{16}$$

characterized by the index σ, that has to be greater than zero to have a square normalizable basis. Each election of σ defines a family of functions which form complete orthonormal set $\mathcal{L}_\sigma$

$$\left\langle \Phi_n^\sigma \middle| \Phi_m^\sigma \right\rangle = \delta_{nm} \tag{17}$$

in the space $L^2[(-1, 1), \mathrm{d}u/(1-u^2)]$ (the square integrable functions on the $(-1, 1)$ interval, with respect to the measure $\mathrm{d}u/(1-u^2)$). This is trivially obtained remembering that the Gegenbauer polynomials $C_n^\kappa(x)$ are orthogonal in the interval $(-1, 1)$ with respect to the weighting function $\omega(x) = (1-x^2)^{\kappa-1/2}$. In principle, we can choose any possible σ to describe the MPT states. The normalization constant in equation (16) is

$$A_n^\sigma = \sqrt{\frac{\alpha n!(\sigma + n - 1/2)[\Gamma(\sigma - 1/2)]^2}{\pi 2^{2-2\sigma}\Gamma(2\sigma + n - 1)}}. \tag{18}$$

In figure 1 the first few basis wavefunctions for a PT potential with $j = 4$ are presented for the election $\sigma = 1$ as a function of the dimensionless quantity αx. In the inset the PT potential is plotted (energies are given in units of $\hbar^2\alpha^2/\mu$). We shall show now that a particular election of σ allows one to decouple the bound states of a given parity from the continuum part of the spectrum.

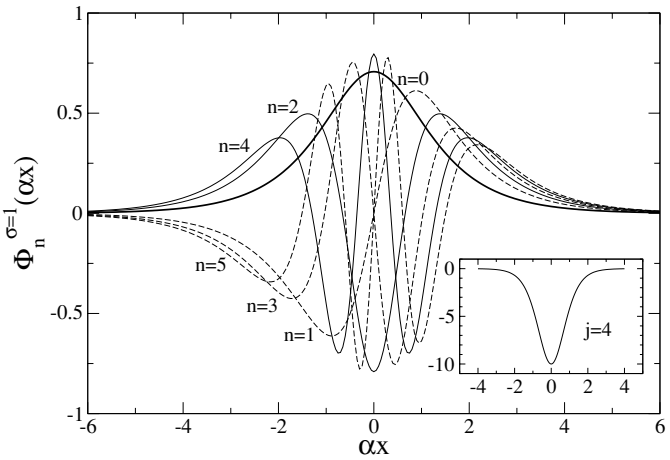

Figure 1. $N = 6$ basis for the Pöschl–Teller potential for the case $\sigma = 1$ (αx is dimensionless). In the inset a Pöschl–Teller potential with $j = 4$ is shown (energy is given in units of $\hbar^2\alpha^2/\mu$).

The MPT Hamiltonian can now be diagonalized in the basis (16) to generate both the discrete and continuum parts of the spectrum. Although this task can be achieved in configuration space [32], we shall follow an algebraic procedure similar to that followed in the case of the Morse potential [38].

In accordance with the factorization method [17, 18], we proceed to obtain the ladder operators for the orthonormalized basis. To this end we start by establishing the action of the differential operator $\frac{\mathrm{d}}{\mathrm{d}u}$ on the functions (16):

$$\frac{\mathrm{d}}{\mathrm{d}u}\Phi_n^\sigma(u) = A_n^\sigma\left\{-\sigma u(1-u^2)^{\sigma/2-1}C_n^{\sigma-1/2}(u) + (1-u^2)^{\sigma/2}\frac{\mathrm{d}}{\mathrm{d}u}C_n^{\sigma-1/2}(u)\right\}. \tag{19}$$

Taking into account the recurrence relations [35]

$$(1-u^2)\frac{\mathrm{d}}{\mathrm{d}u}C_n^\lambda(u) = -(n+1)C_{n+1}^\lambda(u) + (2\lambda+n)uC_n^\lambda(u) \tag{20}$$

$$(n+1)C_{n+1}^\lambda(u) = 2(\lambda+n)uC_n^\lambda(u) - (2\lambda+n-1)C_{n-1}^\lambda(u) \tag{21}$$

and that the momentum in terms of the new variable u is given by $\hat{p} = -\mathrm{i}\hbar\alpha(1-u^2)\,\mathrm{d}/\mathrm{d}u$, we can define the raising, lowering and number operators as

$$\hat{K}_+ = \left[-\frac{\mathrm{i}}{\hbar\alpha}\hat{p} + u(\hat{n}+\sigma-1)\right]\sqrt{\frac{\hat{n}+\sigma+1/2}{\hat{n}+\sigma-1/2}} \tag{22a}$$

$$\hat{K}_- = \left[\frac{\mathrm{i}}{\hbar\alpha}\hat{p} + u(\hat{n}+\sigma)\right]\sqrt{\frac{\hat{n}+\sigma-3/2}{\hat{n}+\sigma-1/2}} \tag{22b}$$

$$\hat{K}_0 = \hat{n}+\sigma-1/2 \tag{22c}$$

with the following action on the basis wavefunctions (16),

$$\hat{K}_+\Phi_n^\sigma(u) = k_+\Phi_{n+1}^\sigma(u) \tag{23a}$$

$$\hat{K}_- \Phi_n^\sigma(u) = k_- \Phi_{n-1}^\sigma(u) \tag{23b}$$

$$\hat{K}_0 \Phi_n^\sigma(u) = k_0 \Phi_n^\sigma(u) \tag{23c}$$

with

$$\hat{k}_+ = \sqrt{(n+1)(2\sigma+n-1)} \tag{24a}$$

$$k_- = \sqrt{n(2\sigma+n-2)} \tag{24b}$$

$$k_0 = (n+\sigma-1/2). \tag{24c}$$

As we can see, the operator $\hat{K}_-$ annihilates the ground state $\Phi_0^\sigma(y)$, as expected from a step-down operator.

We now proceed to study the algebra associated with the operators $\hat{K}_+$ $\hat{K}_-$ and K_0. It is straightforward to show that they satisfy the commutation relations

$$[\hat{K}_+, \hat{K}_-] = -2\hat{K}_0 \qquad [\hat{K}_0, \hat{K}_-] = -\hat{K}_- \qquad [\hat{K}_0, \hat{K}_+] = \hat{K}_+ \tag{25}$$

which correspond to the $su(1,1)$ algebra [39]. We now proceed to identify the quantum numbers $\{\sigma, n\}$ according to their standard representation [40]. The latter is found by examining the formulae for the $su(1,1)$ discrete series representation.

The $SU(1,1)$ group is noncompact [39]. 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 [40, 41]. 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 (25) and the discrete representations D_κ^+ of this group have the standard form

$$\hat{K}_+|\kappa,\mu\rangle = \sqrt{(\mu+\kappa)(\mu-\kappa+1)}|\kappa,\mu+1\rangle \tag{26a}$$

$$\hat{K}_-|\kappa,\mu\rangle = \sqrt{(\mu-\kappa)(\mu+\kappa-1)}|\kappa,\mu-1\rangle \tag{26b}$$

$$\hat{K}_0|\kappa,\mu\rangle = \mu|\kappa,\mu\rangle \tag{26c}$$

where μ can take the values

$$\mu = \kappa, \kappa+1, \ldots \tag{27}$$

for the Bargmann index κ, which characterizes the irreducible representations.

Since the generators (22) satisfy the $su(1,1)$ algebra, we need to establish the connection between $\{\kappa,\mu\}$ and the quantum numbers $\{\sigma,n\}$ in order to recover (26). This goal is accomplished by the identification of μ with the eigenvalue of $\hat{K}_0$ in (22*c*):

$$\mu = \sigma + n - 1/2 \tag{28}$$

and

$$\kappa = \sigma - 1/2. \tag{29}$$

Finally, the Casimir operator can be written as

$$\hat{C} = \hat{K}_+\hat{K}_- - \hat{K}_0(\hat{K}_0 - 1) = \hat{K}_-\hat{K}_+ - \hat{K}_0(\hat{K}_0 + 1) \tag{30}$$

with eigenvalues

$$\hat{C}\Phi_n^\sigma(y) = -\kappa(\kappa-1)\Phi_n^\sigma(y) = -\left[\sigma(\sigma-2) + \tfrac{3}{4}\right]\Phi_n^\sigma(y). \tag{31}$$

Although the operators $\hat{K}_\pm$ are not symmetrical, the unitary representation (26) assures that $\hat{K}_\pm = \hat{K}_\mp^\dagger$ through the matrix elements

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

The asymmetry, and consequently the normalization factors, seems to be necessary in order to reproduce the standard unitary representation. Symmetric expressions for the raising and lowering operators satisfying the $su(1,1)$ algebra, linear in the operator $\hat{n}$, are possible, but they do not lead to the representation (26). Such operators will be introduced in section 4.

We have thus established the algebra associated with the basis (16). These functions are not eigenfunctions of the MPT Hamiltonian, but it is possible to express the Hamiltonian, as well as any dynamical variable in terms of the algebra

$$G_{su(1,1)} = \{\hat{K}_+, \hat{K}_-, \hat{K}_0\}. \tag{32}$$

Consequently, the $su(1,1)$ algebra can be considered as a suitable dynamical algebra for the MPT system in the space generated by the basis $\mathcal{L}_\sigma$. In this algebraic space, the basis (16) takes the simple form

$$\left|\Phi_n^\sigma\right\rangle = G_n^\sigma (\hat{K}_+)^n \left|\Phi_0^\sigma\right\rangle \tag{33}$$

where the normalization constant is given by

$$G_n^\sigma = \sqrt{\frac{1}{n!(2\sigma)_n}}. \tag{34}$$

We should stress the fact that the operator $\hat{K}_+$ in equation (22*a*) depends on the function over which it acts: it is an n-dependent parameter which is well defined as long as the action is carried out over the spaces (16). We now proceed to establish the Hamiltonian in the algebraic space (32).

4. Hamiltonian

In this section we shall write the MPT Hamiltonian in the $su(1,1)$ space. We start by showing that the operators $\hat{K}_+$ and $\hat{K}_-$ can be explicitly expressed in terms of the coordinate u and the momentum $\hat{p} = -\mathrm{i}\hbar\,\mathrm{d}/\mathrm{d}x$. From (22*a*) and (22*b*) we can readily write the explicit form of the momentum and the coordinate u in terms of the $su(1,1)$ generators

$$\hat{p} = \frac{\mathrm{i}\hbar\alpha}{2}\left[\hat{K}_+\sqrt{\frac{1}{(\hat{n}+\sigma-1/2)(\hat{n}+\sigma+1/2)}}(\hat{n}+\sigma) - \hat{K}_-\sqrt{\frac{1}{(\hat{n}+\sigma-1/2)(\hat{n}+\sigma-3/2)}}(\hat{n}+\sigma-1)\right] \tag{35a}$$

$$u = \frac{1}{2}\left[\hat{K}_+\sqrt{\frac{1}{(\hat{n}+\sigma-1/2)(\hat{n}+\sigma+1/2)}} + \hat{K}_-\sqrt{\frac{1}{(\hat{n}+\sigma-1/2)(\hat{n}+\sigma-3/2)}}\right]. \tag{35b}$$

These expressions can be rewritten in a more symmetrical form introducing the operators

$$\hat{A}_\pm = \frac{1}{\sqrt{\hat{K}_0}}\hat{K}_\pm\frac{1}{\sqrt{\hat{K}_0}} \tag{36a}$$

$$\hat{B}_\pm = \sqrt{\hat{K}_0 \mp \tfrac{1}{2}}\hat{A}_\pm\sqrt{\hat{K}_0 \pm \tfrac{1}{2}}. \tag{36b}$$

In terms of these new operators

$$\hat{p} = \frac{i\hbar\alpha}{2}[\hat{B}_+ - \hat{B}_-] \tag{37a}$$

$$u = \frac{1}{2}[\hat{A}_+ + \hat{A}_-]. \tag{37b}$$

On the other hand, since the potential (1) can be rewritten as $V(u) = -D(1-u^2)$, the MPT Hamiltonian can be expressed in the form

$$\hat{H} = \frac{\hat{p}^2}{2\mu} - \frac{D}{\cosh^2(\alpha x)} = \frac{\hat{p}^2}{2\mu} - \frac{\hbar^2\alpha^2}{2\mu} j(j+1)(1-u^2). \tag{38}$$

Carrying out the substitutions of (37) into (38), we obtain

$$\hat{H} = -\frac{\hbar^2\alpha^2}{8\mu}[4j(j+1) + (\hat{B}_- - \hat{B}_+)^2 - j(j+1)(\hat{A}_+ + \hat{A}_-)^2]. \tag{39}$$

The matrix elements of $\hat{H}$ can be easily calculated with the relations

$$\begin{aligned}
\hat{A}_+\Phi_n^\sigma(u) &= \sqrt{\frac{(n+1)(2\sigma+n-1)}{(n+\sigma-1/2)(n+\sigma+1/2)}}\,\Phi_{n+1}^\sigma(u) \\
\hat{A}_-\Phi_n^\sigma(u) &= \sqrt{\frac{n(2\sigma+n-2)}{(n+\sigma-1/2)(n+\sigma-3/2)}}\,\Phi_{n-1}^\sigma(u) \\
\hat{B}_+\Phi_n^\sigma(u) &= (\sigma+n)\hat{A}_+\Phi_n^\sigma(u) \\
\hat{B}_-\Phi_n^\sigma(u) &= (\sigma+n-1)\hat{A}_-\Phi_n^\sigma(u)
\end{aligned} \tag{40}$$

and are given by

$$\begin{aligned}
\langle\Phi_n^\sigma|\hat{H}|\Phi_n^\sigma\rangle = \frac{\hbar^2\alpha^2}{8\mu}\Bigg\{ &\frac{n(2\sigma+n-2)}{(n+\sigma-1/2)(n+\sigma-3/2)}[j(j+1)+(n+\sigma-1)^2] \\
&+ \frac{(n+1)(2\sigma+n-1)}{(n+\sigma-1/2)(n+\sigma+1/2)}[j(j+1)+(n+\sigma)^2] - 4j(j+1)\Bigg\}
\end{aligned} \tag{41a}$$

$$\begin{aligned}
\langle\Phi_{n+2}^\sigma|\hat{H}|\Phi_n^\sigma\rangle = &\frac{\hbar^2\alpha^2}{8\mu}\frac{1}{(n+\sigma+1/2)}\sqrt{\frac{(n+1)(n+2)(2\sigma+n-1)(2\sigma+n)}{(n+\sigma-1/2)(n+\sigma+3/2)}} \\
&\times[j(j+1)-(\sigma+n)(\sigma+n+1)]
\end{aligned} \tag{41b}$$

$$\begin{aligned}
\langle\Phi_{n-2}^\sigma|\hat{H}|\Phi_n^\sigma\rangle = &\frac{\hbar^2\alpha^2}{8\mu}\frac{1}{(n+\sigma-3/2)}\sqrt{\frac{n(n-1)(2\sigma+n-2)(2\sigma+n-3)}{(n+\sigma-1/2)(n+\sigma-5/2)}} \\
&\times[j(j+1)-(\sigma+n-1)(\sigma+n-2)].
\end{aligned} \tag{41c}$$

Since the non-diagonal matrix elements depend on the parameter σ, we look for an adequate choice of this parameter which allows us to decouple the bound states from the continuum, similar to the case of the Morse potential [38]. The form of the Hamiltonian matrix, however, makes clear that this is not possible; only one parameter is available and two matrix elements are to vanish.

The symmetry of the potential implies that the parity is conserved and consequently the space $\mathcal{L}_\sigma$ can be reduced into even and odd subspaces

$$\mathcal{L}_\sigma = \mathcal{L}_\sigma^e \oplus \mathcal{L}_\sigma^o. \tag{42}$$

The diagonalization of the Hamiltonian matrix reduces to the diagonalization of two tridiagonal matrices, one associated with the even functions $\left|\Phi_{2p}^\sigma\right\rangle$ and the other with the odd functions $\left|\Phi_{2p+1}^\sigma\right\rangle$, where p is a non-negative integer. Although it is not possible to find a value of σ to decouple the continuum states from the bound states in both spaces simultaneously, one can find a value of σ_e which decouples even parity states, and a different value of σ_o which decouples odd parity states. Explicitly, if we choose $\sigma_o = j-(2p+1)$, then the state $n = 2p+1$ will not couple to the next odd state, and so the states $n = 1, 3, \ldots, 2p+1$ decouple from the rest. If we take $\sigma_e = j-2p$, then the state with $n = 2p$ does not couple to the next even state, and so the states with $n = 0, 2, \ldots, 2p$ decouple from the rest. Thus, we see that, by choosing the value of $\sigma > 0$ so that $\sigma + n = j$, where n is an even or odd non-negative integer there is a set of even or odd states which decouple from the rest of the basis. The eigenstates of the Hamiltonian in this restricted basis should indeed be bound eigenstates of the Hamiltonian in the complete Hilbert space.

If we take the lowest possible value of σ satisfying $\sigma + n = j$, we maximize the number of states which decouple from the rest. Taking into account the maximum value of v for the bound states (8), we obtain the following conditions on σ in order to obtain the decoupling:

$$\begin{aligned} &\text{Case (a):} \quad [j]\,\text{even} \qquad \sigma_e = j - [j] \quad \text{and} \quad \sigma_o = j - [j] + 1. \\ &\text{Case(b):} \quad [j]\,\text{odd} \qquad \sigma_e = j - [j] + 1 \quad \text{and} \quad \sigma_o = j - [j]. \end{aligned} \tag{43}$$

If j is fixed there are $[j]+1$ bound states $\Psi_v^j(u)$, characterized by the values of $v = 0, 1, \ldots, [j]$. The parity of v determines the parity of the state. If the values of σ are chosen as σ_e or σ_o, the exact bound states (2) satisfy the following orthogonality condition

$$\left\langle \Psi_v^j \middle| \Phi_n^\sigma \right\rangle = 0 \qquad \forall n > [j]. \tag{44}$$

In the next section we shall prove the orthogonality relations (44). However, one can justify it from the following argument. Let us assume that $[j]$ is even. Then, the MPT Hamiltonian has $[j]/2+1$ bound eigenstates with even parity and $[j]/2$ states with odd parity, which are the only normalizable states of the MPT Hamiltonian in the complete Hilbert space. By taking $\sigma_e = j - [j]$, we get that the states characterized by $n = 0, 2, \ldots, [j]$ decouple from the rest, and so the eigenstates of the Hamiltonian in this basis should also be eigenstates of the Hamiltonian in the complete space. But these eigenstates are $[j]/2+1$, and are normalizable. So, they should be the even parity eigenstates of the Hamiltonian. Hence, the states with $n > [j]$, which are orthogonal to the states with $n \leqslant [j]$, must also be orthogonal to the bound states with positive parity. The same argument can be applied for the odd parity states. When $[j]$ is odd, we will get $([j]+1)/2$ odd parity states and $([j]+1)/2$ even parity states, but the argument is essentially the same.

As an example, we present in figure 2 the eigenstates obtained for the MPT Hamiltonian with $j = 4$ as the dimension of the basis is enlarged from 4 to 20. Here we have selected $\sigma = 1$, in this case the bound odd parity states are decoupled from the rest. The inset is a zoom of the low energy part, it is seen that the states $n = 1$ and $n = 3$ have the exact energy in all the cases as expected. The energies of the states with $n = 0$ and $n = 2$ are not the exact ones in principle, but the overlaps with the exact states are large with a small basis. For example, in the case of a basis with $N = 6$ (3 even and 3 odd states) the overlaps of those states with the exact ones are 99.998% and 98.833% respectively. Energies are given in units of $\hbar^2\alpha^2/\mu$. It is seen that when adding one state to the basis the states of the other parity remain of the same energy, since the parity is a good quantum number here.

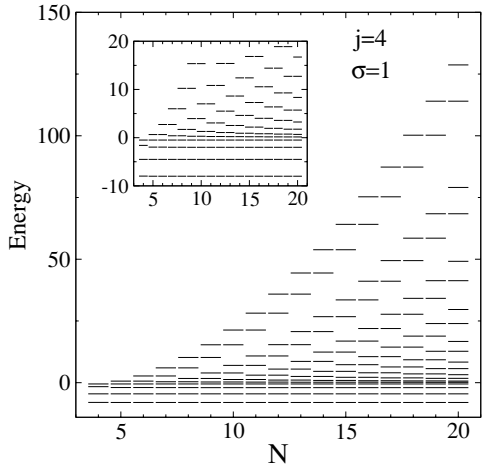

Figure 2. Energy eigenvalues (dimensionless, in units of $\hbar^2\alpha^2/\mu$), for the Pöschl–Teller potential with $j = 4$ as a function of the size of the basis N generated for $\sigma = 1$. The inset is a zoom of the low energy region.

5. Interpretation of the basis $\Phi_n^\sigma(u)$

In order to interpret the family of orthonormal functions (16) we need to introduce the raising and lowering operators in the framework of the potential group approach [42]. We thus look for operators that shift the number of quanta as well as the potential parameter j.

Applying the operator $(1-u^2)\frac{\mathrm{d}}{\mathrm{d}u}$ to (2), and using relation (20), we obtain

$$(1-u^2)\frac{\mathrm{d}}{\mathrm{d}u}\Psi_v^j(u) = u(j+1)\Psi_v^j(u) - (v+1)\frac{N_v^j}{N_{v+1}^{j+1}}\Psi_{v+1}^{j+1}(u) \tag{45}$$

where we have introduced the identification

$$\Psi_{v+1}^{j+1}(u) = N_{v+1}^{j+1}(1-u^2)^{\frac{j-v}{2}}C_{v+1}^{j-v+1/2}(u). \tag{46}$$

So, the state $\Psi_{v+1}^{j+1}(u)$ is the bound eigenstates with $v+1$ quanta of a MPT potential whose depth is characterized by $j+1$.

At this point we introduce the operators

$$\hat{M}_\pm(q) = \mp(1-u^2)\frac{\mathrm{d}}{\mathrm{d}u} + qu \tag{47}$$

which have the remarkable property that can be expressed in terms of a linear combination of operators $\hat{M}_\pm(q')$ with different arguments

$$\hat{M}_\pm(q) = \frac{q+q''}{q'+q''}\hat{M}_\pm(q') + \frac{q-q'}{q'+q''}\hat{M}_\mp(q''). \tag{48}$$

We note that the raising or lowering operators with different arguments do not commute. In particular, we shall be interested in the commutation relation

$$[\hat{M}_+(q), \hat{M}_+(q')] = (q'-q)(1-u^2). \tag{49}$$

Taking into account the appropriate recurrence relations for the Geguenbauer polynomials, we obtain without difficulty the action of the operators (47) for particular values of q on the wavefunctions

$$\hat{M}_-(j)\Psi_v^j(u) = \sqrt{v(2j-v)}\,\Psi_{v-1}^{j-1}(u) \tag{50a}$$

$$\hat{M}_+(j+1)\Psi_v^j(u) = \sqrt{(v+1)(2j-v+1)}\,\Psi_{v+1}^{j+1}(u). \tag{50b}$$

On the other hand, comparing the operators (47) with $\hat{K}_\pm$ given by (22*a*), (22*b*), we note that they differ by a normalization factor only, a fact that allows us to obtain the action of the operators $\hat{M}_\pm$ on the basis (16):

$$\hat{M}_-(\sigma+n)\Phi_n^\sigma(u) = \sqrt{\frac{n(\sigma+n-1/2)(2\sigma+n-2)}{(\sigma+n-3/2)}}\,\Phi_{n-1}^\sigma(u) \tag{51a}$$

$$\hat{M}_+(\sigma+n-1)\Phi_n^\sigma(u) = \sqrt{\frac{(n+1)(\sigma+n-1/2)(2\sigma+n-1)}{(\sigma+n+1/2)}}\,\Phi_{n+1}^\sigma(u). \tag{51b}$$

Consequently, the action of the generalized operators $\hat{M}_\pm(q)$ on both the bound MPT wavefunctions (2) and the basis functions (16) is known.

From the definition of $\hat{M}_+(q)$ we can write the MPT wavefunctions in terms of successive application of appropriate $\hat{M}_+$ operators over $\Psi_0^{j-v}(u)$,

$$\left|\Psi_v^j\right\rangle = D_v^j \prod_{\beta=1}^{v} \hat{M}_+(j-v+\beta)\left|\Psi_0^{j-v}\right\rangle \tag{52}$$

where

$$D_v^j = \sqrt{\frac{1}{v!\,(2j-2v+1)_v}}. \tag{53}$$

In addition, from equations (2) and (16), the following relation is obtained,

$$\left|\Psi_0^{j-v}\right\rangle = C(j,v,\sigma)(1-u^2)^{\frac{j-v-\sigma}{2}}\left|\Phi_0^\sigma\right\rangle \tag{54}$$

where

$$C(j,v,\sigma) = \frac{N_0^{j-v}}{A_0^\sigma}. \tag{55}$$

Taking into account the possible values of σ given in (43), we find that $j-v-\sigma$ is a non-negative integer corresponding to the number of bound states higher in energy than $\left|\Psi_v^j\right\rangle$ with the same parity of v. The substitution of (54) into (52), using (49), gives rise to the expression

$$\left|\Psi_v^j\right\rangle = E(j,v)\left(\prod_{\beta=1}^{v}\hat{M}_+(j-v+\beta)\right)[\hat{M}_+(\sigma),\hat{M}_+(\sigma-1)]^{\frac{j-v-\sigma}{2}}\left|\Phi_0^\sigma\right\rangle \tag{56}$$

where

$$E(j,v) = C(j,v,\sigma)D_v^j. \tag{57}$$

It can be seen that this expression contains at maximum a number of $\hat{M}_+$ operators corresponding to the total number of bound states, which is equal to $[j]$ or $[j]-1$, depending on the parity of v.

In the same way, from equations (51) we can write the basis wavefunctions $\Phi_n^\sigma(u)$ in terms of successive applications of $\hat{M}_+$ over $\Phi_0^\sigma(u)$,

$$\left|\Phi_n^\sigma\right\rangle = B_n^\sigma \prod_{\beta=1}^{n}\hat{M}_+(\sigma-2+\beta)\left|\Phi_0^\sigma\right\rangle. \tag{58}$$

We next come back to the selection rule (44), but now from the point of view of the new operators (47). The expansion of the commutator in (56) generates a sum of products of operators $\hat{M}_+$ with $j - v - \sigma$ factors. If we add the effect of the v operators indicated in parentheses in (56), a linear combination of products of operators $\hat{M}_+$ with a number of factors corresponding to $[j]$ or $[j]+1$, depending on the parity of v, is generated. The effect over the state $\left|\Psi_0^\sigma\right\rangle$ of each sequence of $[j]$ (or $[j]-1$) products of operators $\hat{M}_+(q)$ is obtained by using (48), in such a way that selecting appropriately the arguments q' and q'' they increase or decrease the index ζ in the basis $\left|\Phi_\zeta^\sigma\right\rangle$. As a result the eigenfunctions $\left|\Psi_v^j\right\rangle$ are given in terms of a linear combination of functions $\left|\Phi_\zeta^\sigma\right\rangle$ with $\zeta = 0, 1, \ldots, [j]$ or $[j]-1$. Finally, because of the property (17), the orthogonality (44) is satisfied.

We next show the relation of the present approach to the potential approach and the supersymmetric quantum mechanics treatment. Comparing the forms of the bound MPT wavefunctions (2) and the family of orthonormal functions (16) and using the known relation for the Gegenbauer polynomials

$$(n+\alpha)C_{n+1}^{\alpha-1}(x) = (\alpha-1)\left(C_{n+1}^{\alpha}(x) - C_{n-1}^{\alpha}(x)\right) \tag{59}$$

it is obtained rightaway that

$$\left|\Phi_n^\sigma\right\rangle = S_n^\sigma\left[\sqrt{(2\sigma+n)(2\sigma+n-1)}\left|\Psi_n^{\sigma+n}\right\rangle - \sqrt{n(n-1)}\left|\Psi_{n-2}^{\sigma+n-2}\right\rangle\right] \tag{60}$$

with

$$S_n^\sigma = \frac{1}{2\sqrt{\sigma(n+\sigma-1/2)}}. \tag{61}$$

The family of functions $\Phi_n^\sigma(u)$ are then a linear combination of MPT-like functions with potential parameters $\sigma+n$ and $\sigma+n-2$. This result explains the resemblance of the operators (47) with the operators obtained in the potential approach. The functions (16) turn out to be MPT-like functions associated with different potential depths.

Concerning the supersymmetric quantum mechanics approach, we should note that the MPT Hamiltonian can be factorized in the form

$$\hat{H} = \frac{\hbar^2\alpha^2}{2\mu}[\hat{M}_+(j)\hat{M}_-(j) - j^2] \tag{62}$$

an expression which is derived from supersymmetric quantum mechanics [5]. The matrix elements of this operator in the basis $\left|\Phi_n^\sigma\right\rangle$ are obtained by means of the transformations (48) which, when applied to (62), lead to the matrix elements (41). The connection of the operators $\hat{M}_\pm$ with the factorization (62) is a consequence of the relation between the factorization method and the concept of shape invariant potentials discussed in supersymmetric quantum mechanics [43].

6. Dipole function

Once the Hamiltonian has been diagonalized we obtain the energy spectrum as well as the eigenfunctions. The quality of the energies is estimated by the calculation of the root mean square deviation. In general, however, a good description of the energy spectrum is not necessarily accompanied by high quality of the eigenstates. It is thus compulsory to evaluate the goodness of the eigenfunctions through the calculation of other observables. One of the most important observables is the dipole transition intensity. We shall thus present a discussion of matrix elements of the dipole operator.

Since in general the form of the dipole function is not known, it is common to express the dipole function as a Taylor series expansion around the equilibrium positions. This expansion

must take into account the symmetry properties of the system. For a one-dimensional system the dipole function carries the odd irreducible representation. Since the natural variable for the Pöschl–Teller potential is $u = \tanh(\alpha x)$, we propose the expansion

$$\mu(x) = \sum_{p=0}^{P} \frac{u^{2p+1}}{(2p+1)!} \left(\frac{\mathrm{d}^{2p+1}\mu}{\mathrm{d}u^{2p+1}} \right)_e \tag{63}$$

where we have considered a finite sum and have taken into account the odd character of both the dipole function and the variable u.

We thus intend to obtain the matrix elements

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

which implies the calculation of the matrix elements

$$M_{mn}^{2p+1} = \left\langle \Phi_m^\sigma \middle| \hat{u}^{2p+1} \middle| \Phi_n^\sigma \right\rangle. \tag{65}$$

The matrix elements (65) can be obtained by means of recurrence relations. The seeds for such relations are the matrix elements

$$\left\langle \Phi_{n+1}^\sigma \middle| u \middle| \Phi_n^\sigma \right\rangle = \frac{1}{2} \sqrt{\frac{(n+1)(2\sigma+n-1)}{(\sigma+n-1/2)(\sigma+n+1/2)}} \tag{66a}$$

$$\left\langle \Phi_{n-1}^\sigma \middle| u \middle| \Phi_n^\sigma \right\rangle = \frac{1}{2} \sqrt{\frac{n(2\sigma+n-2)}{(\sigma+n-1/2)(\sigma+n-3/2)}}. \tag{66b}$$

Introducing the closure relation

$$\sum_\beta \left| \Phi_\beta^\sigma \right\rangle \left\langle \Phi_\beta^\sigma \right| = 1 \tag{67}$$

the matrix elements (65) can be rewritten as

$$\left\langle \Phi_m^\sigma \middle| u^{2p+1} \middle| \Phi_n^\sigma \right\rangle = \sum_\beta \left\langle \Phi_m^\sigma \middle| u^{2p-1} \middle| \Phi_\beta^\sigma \right\rangle \left\langle \Phi_\beta^\sigma \middle| u^2 \middle| \Phi_n^\sigma \right\rangle \qquad p = 1, 2, \ldots \tag{68}$$

where

$$\left\langle \Phi_\beta^\sigma \middle| u^2 \middle| \Phi_n^\sigma \right\rangle = \left\langle \Phi_\beta^\sigma \middle| u \middle| \Phi_{n+1}^\sigma \right\rangle \left\langle \Phi_{n+1}^\sigma \middle| u \middle| \Phi_n^\sigma \right\rangle + \left\langle \Phi_\beta^\sigma \middle| \hat{u} \middle| \Phi_{n-1}^\sigma \right\rangle \left\langle \Phi_{n-1}^\sigma \middle| \hat{u} \middle| \Phi_n^\sigma \right\rangle \tag{69}$$

with $\beta = n, n \pm 2$. Taking into account this result, expression (68) can be recast into the explicit form

$$\begin{aligned} \left\langle \Phi_{n\pm(2\alpha+1)}^\sigma \middle| \hat{u}^{2p+1} \middle| \Phi_n^\sigma \right\rangle &= \left\langle \Phi_{n\pm(2\alpha+1)}^\sigma \middle| \hat{u}^{2p-1} \middle| \Phi_n^\sigma \right\rangle \left\langle \Phi_n^\sigma \middle| \hat{u}^2 \middle| \Phi_n^\sigma \right\rangle \\ &+ \left\langle \Phi_{n\pm(2\alpha+1)}^\sigma \middle| \hat{u}^{2p-1} \middle| \Phi_{n+2}^\sigma \right\rangle \left\langle \Phi_{n+2}^\sigma \middle| \hat{u}^2 \middle| \Phi_n^\sigma \right\rangle \\ &+ \left\langle \Phi_{n\pm(2\alpha+1)}^\sigma \middle| \hat{u}^{2p-1} \middle| \Phi_{n-2}^\sigma \right\rangle \left\langle \Phi_{n-2}^\sigma \middle| \hat{u}^2 \middle| \Phi_n^\sigma \right\rangle \end{aligned} \tag{70}$$

where the matrix elements involving odd powers of u satisfy

$$\left\langle \Phi_{n\pm(2\alpha+1)}^\sigma \middle| u^{2p-1} \middle| \Phi_{n+\gamma}^\sigma \right\rangle \neq 0 \qquad \text{if} \quad |\pm(2\alpha+1) - \gamma| \leqslant 2p+1 \tag{71}$$

for $\gamma = 0, \pm 2$. Starting with the matrix elements (66) we can generate the matrix elements of any (odd) power of u using (70) and consequently the dipole matrix elements (63).

As an illustration of the results that can be obtained we have done a simple calculation using a dipole operator function

$$\hat{\mu}(x) = u(1 - u^2) \tag{72}$$

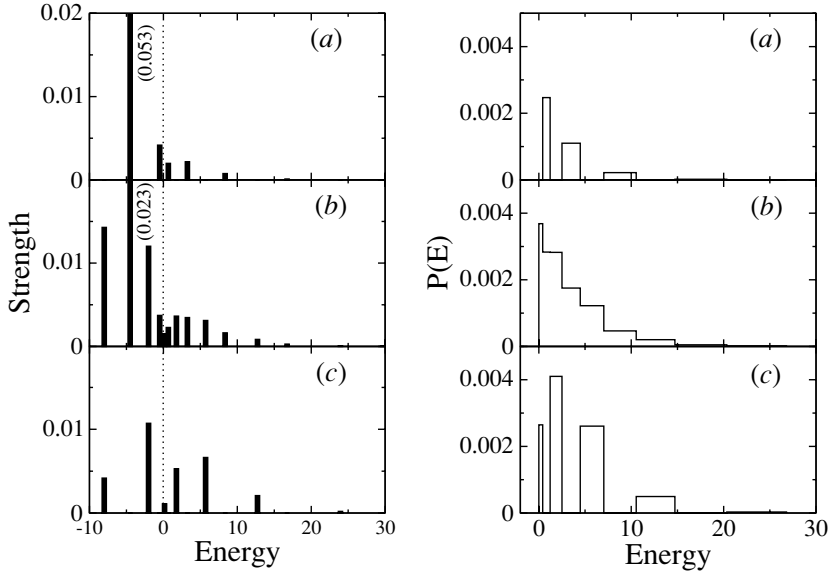

Figure 3. Transition strength to all states (left panels) and probability density for transitions to the continuum (right panels) from the ground state (*a*), from an average with equal weights of all bound states (*b*) and from the least bound state (*c*). The diagonal terms are also included. The dipole operator used is given in equation (72). The calculation is done with a basis generated for $\sigma = 1$ of $N = 20$ states for a Pöschl–Teller potential with $j = 4$. The probability density to the continuum is represented as a histogram as explained in the text.

where $u = \tanh(x)$. We use dimensionless magnitudes in such a way that energies are given in units of $\hbar^2\alpha^2/\mu$ and distances are given in units of α^{-1}. The calculations presented are for a MPT Hamiltonian with $j = 4$ and with the election $\sigma = 1$. We 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. Left panels give transition strengths starting from different initial state: in the upper 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 ($n = 3$). Right panels are 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 we represent it as a histogram. Due to parity the strength from the state $n = 0$ goes only to odd parity states in the continuum, while the strength from $n = 3$ goes only to even parity states. This selection rule does not apply to the middle panel since the initial state is an average including both even and odd parity bound states. It can be seen that the maximum of the distribution moves up in energy as the initial state is less bound and that 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

Table 1. Convergence of the total strength (S) and energy weighted sum rule (E_W) to the continuum for the operator $\hat{\mu} = u(1-u^2)$ as a function of the discrete basis dimension generated for $\sigma = 1$ for the Pöschl–Teller Hamiltonian with $j = 4$. Two cases are presented: one with the ground state as initial and the other with the least bound state as initial. 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	0.004 8805	0.052 369	0.005 2729	0.006 0102
8	0.005 0430	0.057 189	0.015 603	0.085 813
10	0.005 0263	0.056 859	0.015 407	0.086 213
20	0.005 0239	0.056 850	0.015 306	0.086 415
Exact value	0.005 0239	0.056 850	0.015 301	0.086 424

($n = 0$) and the least bound state ($n = 3$). Table 1 shows that for the case starting in the ground state the convergence is fast and already with $N = 20$ (8 even and 8 odd states in the continuum plus the 4 bound states) the exact values for both the total strength and the energy weighted sum rule are obtained. For the least favourable case starting in $n = 3$ a basis of $N = 20$ states provides an extremely good approximation to the exact values.

We have investigated the one-dimensional case, for which the dipole function has a definite parity. In three-dimensional problems, however, the dipole function is a vector whose components may carry several irreducible representations. As a consequence, even powers of the variable u may be involved. Let us consider an example. Formaldehyde (CH_2O) is a planar molecule with one mode out-of-plane. In a local mode description a possible set of internal coordinates to be chosen is the two distances CH (r_1, r_2) , the distance CO (r_3) and the two angles $\angle$HCO (θ_1, θ_2). Finally, from the dihedral angle γ between the normal of the planes defined by the two sets of HCO atoms, the out-of-plane bending angle coordinate $\delta = \gamma - \pi$ is defined. The dipole function carries the irreducible representations B_1, B_2 and A_1, for the x, y and z components, respectively. Choosing the molecule in the xz plane, the dihedral angle spans the B_2 representation. The dipole function may thus be expanded in terms of this set of internal coordinates, but a better alternative is represented by symmetry adapted coordinates. If we define the coordinates

$$S_s^{A_1} = \frac{1}{\sqrt{2}}(r_1 + r_2) \tag{73a}$$

$$S_s^{A_2} = \frac{1}{\sqrt{2}}(r_1 - r_2) \tag{73b}$$

$$Q_s^{A_1} = r_3 \tag{73c}$$

$$S_b^{A_1} = \frac{1}{\sqrt{2}}(\theta_1 + \theta_2) \tag{73d}$$

$$S_b^{A_2} = \frac{1}{\sqrt{2}}(\theta_1 - \theta_2) \tag{73e}$$

$$S_o^{B_2} = u \tag{73f}$$

where $u = \tanh(\alpha\delta)$ and s, b stand for stretching and bending, respectively. The components of the dipole moment are represented as [44]

$$\mu_\alpha^\Gamma = \sum_{ijklmn} \mu_{ijklmn}^{\Gamma,\alpha} \left(S_s^{A_1}\right)^i \left(S_s^{A_2}\right)^j \left(Q_s^{A_1}\right)^k \left(S_b^{A_1}\right)^l \left(S_b^{A_2}\right)^m \left(S_o^{B_2}\right)^n \tag{74}$$

where $\Gamma = B_1, B_2, A_1$ and $\alpha = x, y, z$, respectively, while the coefficients $\mu_{ijklmn}^{\Gamma,\alpha}$ are related to the derivatives of the dipole evaluated in the equilibrium. In (74) the allowed powers in the sum are restricted to satisfy

$$\Gamma = (A_1)^i \otimes (A_2)^j \otimes (A_1)^k \otimes (A_1)^l \otimes (A_2)^m \otimes (B_2)^n. \tag{75}$$

For terms in the expansion (74) with $i = j = k = l = m = 0$, the non-vanishing coefficients are

$$\mu_{00000n}^{A_1,z} \neq 0 \qquad n \text{ even} \tag{76}$$

$$\mu_{00000n}^{B_2,y} \neq 0 \qquad n \text{ odd} \tag{77}$$

as expected from (75). We thus have to obtain a recurrence relation to generate the matrix element with even powers of u. Such a relation can be obtained in a straightforward way and is given by

$$\langle \Phi_m^\sigma | u^{2p} | \Phi_n^\sigma \rangle = \langle \Phi_m^\sigma | u^{2p-1} | \Phi_{n+1}^\sigma \rangle \langle \Phi_{n+1}^\sigma | u | \Phi_n^\sigma \rangle + \langle \Phi_m^\sigma | \hat{u}^{2p-1} | \Phi_{n-1}^\sigma \rangle \langle \Phi_{n-1}^\sigma | \hat{u} | \Phi_n^\sigma \rangle. \tag{78}$$

We can thus obtain the matrix elements with even powers of u in terms of the matrix elements previously generated for the odd powers.

7. Summary and conclusions

In this work we have proposed a complete set of functions to describe both the bound and continuum parts of the spectrum for the MPT potential. We have shown that the ladder operators for this set of functions satisfy the $su(1, 1)$ commutation relations, a fact that leads us to consider the $su(1, 1)$ algebra as a dynamical algebra of the MPT. This analysis allows us to approach the description in terms of an algebraic formalism, which considerably simplifies the calculations. A remarkable result of this analysis is that it is possible to decouple the bound states from the continuum either for the even or the odd parity states. For the parity where the decoupling is not carried out, the exact bound eigenvalues are recovered with a relatively small basis. The potential approach is used to interpret the basis (16), which turns out to be linear combinations of MPT-like functions with different potential depths. Recurrence relations for the calculation of the dipole matrix elements are established.

In a local mode description for molecular vibrational excitations the MPT potential is suitable to describe the out-of-plane modes. With the advent of new spectroscopic techniques [45–47], excitations with a high number of quanta in the out-of-plane modes can be obtained. When the excitation energies are near the dissociation barrier, the continuum may play a preponderant role, and consequently should not be neglected. We believe that the model we propose will be useful to deal with these situations.

Acknowledgments

This work is partially supported by DEGAPA-UNAM, Mexico, under project IN101302, CONACyT, Mexico, and DGI, Spain, under projects BFM2002-03315 and FPA2002-04181-C04-04.

References

[1] Wigner E P 1959 *Group Theory in its Applications to the Quantum Mechanics of Atomic Spectra* (New York: Academic)

[2] Dutt R, Khare A and Sukhatme U P 1988 *Am. J. Phys.* **56** 163
[3] Pöschl G and Teller E Z 1933 *Z. Phys.* **83** 143
[4] Rosen N and Morse P M 1932 *Phys. Rev.* **42** 210
[5] Cooper F, Khare A and Sukhatme U P 1995 *Phys. Rep.* **251** 268
[6] Frank A and Wolf K B 1984 *Phys. Rev. Lett.* **52** 1737
[7] Alhassid Y, Engel J and Iachello F 1986 *Phys. Rev. Lett.* **57** 9
[8] Hornburger H and Dierckensen G H F 1998 *J. Math. Chem.* **24** 39
[9] Bagchi B, Mallik S and Quesne C 2001 *Int. J. Mod. Phys.* **16** 2859
[10] Bagchi B and Quesne C 2000 *Phys. Lett.* A **273** 285
[11] Bagchi B, Mallik S and Quesne C 2002 *Int. J. Mod. Phys.* **17** 51
[12] Zúñiga J, Alacid M, Requena A and Bastida A 1996 *Int. J. Quantum Chem.* **57** 43
[13] Nieto M M 1978 *Phys. Rev.* A **17** 1263
[14] Dong S H and Lemus R 2002 *Int. J. Quantum Chem.* **86** 265
[15] Lemus R and Bernal R 2002 *Chem. Phys.* **283** 401
[16] Frank A and Van Isacker P 1994 *Algebraic Methods in Molecular and Nuclear Structure Physics* (New York: Wiley)
[17] Schrödinger E 1940 *Proc. R. Ir. Acad.* A **46** 183
[18] Infeld L and Hull T E 1951 *Rev. Mod. Phys.* **23** 21
[19] Choi Y S and Moore C B 1993 *J. Chem. Phys.* **110** 1111
[20] Child M S and Lawton R T 1981 *Faraday Discuss Chem. Soc.* **71** 273
[21] Child M S and Halonen L 1984 *Adv. Chem. Phys.* **1** 1
[22] Halonen L 1998 *Adv. Chem. Phys.* **104** 41
[23] Jensen P 2000 *Mol. Phys.* **98** 1253
[24] Lemus R, Carvajal M, López-V J C and Frank A 2002 *J. Mol. Spectrosc.* **214** 52
[25] Wigner E P and Eisenbud L 1947 *Phys. Rev.* **72** 29
Burke P G and Berrington K A (ed) 1993 *Atomic and Molecular Processes: An R-Matrix Approach* (Bristol: Institute of Physics Publishing)
[26] Rotenberg M 1970 *Adv. At. Mol. Phys.* **6** 233
[27] Antonsen F 1999 *Phys. Rev.* A **60** 812
[28] Szmytkowski R and Zywicka-Mozejko B 2000 *Phys. Rev.* A **62** 022104
[29] Tolstikhin O I, Ostrovsky V N and Nakamura H 1998 *Phys. Rev.* A **58** 2077
[30] Lovas R G, Liotta R J, Insolia A, Varga K and Delion D S 1998 *Phys. Rep.* **294** 265
[31] Austern N, Iseri Y, Kamimura M, Kawai M, Rawitsher G and Yahiro M 1987 *Phys. Rep.* **154** 125
[32] Pérez-Bernal F, Martel I, Arias J M and Gómez-Camacho J 2001 *Phys. Rev.* A **63** 052111
[33] Flügge S 1971 *Practical Quantum Mechanics* (Berlin: Springer)
[34] Landau L D and Lifshitz E M 1977 *Quantum Mechanics* (Oxford: Pergamon)
[35] Gradshteyn I S and Ryzhik I M 1994 *Tables of Integrals, Series, and Products* 5th edn (New York: Academic)
[36] Rose M E 1995 *Elementary Theory of Angular Momentum* (New York: Dover)
[37] Van Roosmalen O S, Benjamin I and Levine R D 1984 *J. Chem. Phys.* **81** 5986
[38] Lemus R, Arias J M and Gómez-Camacho J An $su(1, 1)$ dynamical group for the Morse potential *J. Phys. A: Math. Gen.* to be published
[39] Wybourne R G 1974 *Classical Groups for Physicists* (New York: Wiley)
[40] Bargmann V 1947 *Ann. Math.* **48** 568
[41] Perelomov A 1985 *Generalized Coherent States and their Applications* (New York: Springer)
[42] Cooper I L 1993 *J. Phys. A: Math. Gen.* **26** 1601
[43] Alves N A and Filho D 1988 *J. Phys. A: Math. Gen.* **18** 3215
[44] Poulin N M, Bramley M J, Carrington T Jr, Kjaergaard H G and Henry B R 1996 *J. Chem. Phys.* **104** 7807
[45] Hollas J M 1998 *High Resolution Spectroscopy* (New York: Wiley)
[46] Kittrell C 1995 *Stimulated Emission Pumping by Fluorescence Dip: Experimental Methods, Molecular Dynamics and Spectroscopy by Stimulated Emission Pumping* (New Jersey: World Scientific)
[47] Dai H-L and Field R W 1995 *Molecular Dynamics and Spectroscopy by Stimulated Emission Pumping* (Singapore: World Scientific)