Ladder Operators for the Morse Potential

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ABSTRACT: A realization of the raising and lowering operators for the Morse potential is presented. It is shown that these operators satisfy the commutation relations for the SU(2) group. Closed analytical expressions are obtained for the matrix elements of different operators such as $1/y$ and d/dy. The harmonic limit of the SU(2) operators is also studied and an approach previously proposed to calculate the Franck–Condon factors is discussed. Int J Quantum Chem 86: 433–439, 2002

Key words: ladder operators; SU(2) group; Morse potential

Introduction

The study of exactly solvable problems has attracted much attention since the early development of quantum mechanics. A fundamental work in this direction was made by Schrödinger [1], who introduced the factorization method. This approach was generalized by Infeld and Hull [2] and others [3], where a detailed analysis of factorizable potentials was presented. The application of the factorization method leads to the description of the systems in terms of creation and annihilation operators, which together with other operators may close into an algebra. Related with this approach is the supersymmetry transformation [4–6], which was recognized by Gendenshtein [7] to be closely connected to solvable potentials. He introduced the concept of shape invariance and proved that when satisfied the wave functions could be determined by purely algebraic means. By using this method it was possible to obtain explicit wave functions for all known shape-invariant potentials [8]. In addition, it was shown that shape invariance has an underlying algebraic structure associated to Lie algebras [9, 10].

Because of its importance in the field of molecular physics [11–13], the Morse potential has been the subject of many studies. This potential is solvable, hence the interest is to deal with it using different approaches, in particular factorization methods [8, 9, 14]. On the basis of these methods an SU(1,1) algebra has been identified [9, 15, 16]. On the other hand, it is known that SU(2) is the dynamical group associated with the bounded region of the spectrum [17]. Therefore a natural question concerns the explicit construction of the SU(2) generators and their relation to the ladder operators of the Morse system.

The Morse potential has been studied both in terms of the SO(2,1) [18–23] and SU(2) groups [24, 25]. The latter description has been exploited in

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the development of an algebraic treatment of molecular vibrations in polyatomic molecules, which incorporates anharmonic effects at the local mode level, while the former turned out to be relevant for the algebraic determination of S matrices under scattering conditions. The fundamental difference between these approaches is that SO(2,1) is a noncompact group, which involves either unitary continuous representations or infinite-dimensional discrete ones. Thus the raising and lowering operators of SO(2,1) are associated with step variations of the potential depth, keeping a fixed energy [15], while the SU(2) formulation involves the description of the bound states only, a finite number [24, 25]. While in SO(2,1) the Morse Hamiltonian is associated to the Casimir invariant (the potential group approach [26–29]), in the case of SU(2) the Hamiltonian is a simple function of the generators [17, 24]. The connection of the SU(2) group with the Morse system can be directly established by means of a coordinate transformation applied on the two-dimensional (2D) radial equation of the harmonic oscillator. This procedure, however, does not provide us with an explicit realization of the SU(2) generators in terms of the "physical" coordinate. This realization was explored further in [30, 31], where a comparison of Morse matrix elements with those of SU(2) leads to a series expansion of the coordinate and momentum in terms of the SU(2) generators. Other investigations have used a realization of these operators that involve an auxiliary variable [17], while Nieto and Simmons constructed raising and lowering operators that were not, however, linked with a group structure [32].

Recently, Avram and Drăgănescu [33] established a realization of the raising and lowering operators of the Morse potential, basing their approach on some properties of the confluent hypergeometric functions. They claimed that these operators, together with a number operator, satisfy the commutation relations of the SO(2,1) group and proposed an algebraic method to establish recurrence relations for the Franck–Condon factors. Although the basic idea is correct, we show in this study that the derivation is flawed. As we indicate below, their use of integral representations for the confluent hypergeometric functions is invalid. In addition, the normalization integrals were taken incorrectly and thus their conclusions cannot be sustained. Most importantly, our analysis leads to the SU(2) group and not to the noncompact SO(2,1) one. As explained above, this is the natural group structure to expect for the description of the finite number of bound states sustained by the Morse oscillator, in accordance with previous studies [17].

The aim of this study is twofold. On the one hand, we derive a new realization of the step generators for the Morse potential using an algebraic method and show that together with a weight generator they exactly satisfy the SU(2) commutation relations. We verify our results by calculating matrix elements of certain functions of the Morse coordinate and momentum, and study the harmonic limit, and indicate some other possible applications of these operators. On the other hand, we show that subsequent work using the results of Ref. [33] must be revised and, in particular, that the calculation of Franck–Condon factors through linear recurrence relations lacks generality and can only be used in very particular cases.

This study is organized as follows. In the following section, we establish the raising and lowering operators directly from the eigenfunction of the Morse potential with the factorization method [1–3]. The matrix elements of the operators $1/y$ and d/dy are obtained with the aid of these operators. The third section is devoted to show how the harmonic limit is attained. We then present arguments leading to the conclusion that the approach proposed in [33] to compute the Franck–Condon factors is not general. In the final section we present our summary and conclusions.

Ladder Operators for the Morse Potential

Choosing the separated atoms limit as the zero of energy, the Morse potential has the following form [34]:

$$V(x) = V_0\left(e^{-2\beta x} - 2e^{-\beta x}\right), \tag{1}$$

where $V_0 > 0$ corresponds to its depth, β is related with 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 to the Morse potential is given by [35]:

$$\Psi_n^\nu(y) = N_n^\nu e^{-y/2} y^s L_n^{2s}(y), \tag{2}$$

where $L_n^{2s}(y)$ are the associated Laguerre functions, the argument y is related with the physical displacement coordinate x by $y = \nu e^{-\beta x}$, and N_n^ν is the normalization constant:

$$N_n^\nu = \sqrt{\frac{\beta(\nu - 2n - 1)\Gamma(n+1)}{\Gamma(\nu - n)}}, \tag{3}$$

and the variables ν and s are related with the potential and the energy, respectively, through

$$\nu = \sqrt{\frac{8\mu V_0}{\beta^2\hbar^2}}, \qquad s = \sqrt{\frac{-2\mu E}{\beta^2\hbar^2}}, \tag{4}$$

with the constraint condition $2s = \nu - 2n - 1$, where μ is the reduced mass of the molecule.

In this section we address the problem of finding creation and annihilation operators for the Morse wave functions (2) using the basic ideas proposed by Avram and Drăgănescu [33], but following a different approach. In other words, we intend to find differential operators $\hat{\mathcal{O}}_\pm$ with the following property:

$$\hat{\mathcal{O}}_\pm \Psi_n^\nu(y) = o_\pm \Psi_{n\pm1}^\nu(y). \tag{5}$$

Specifically, we look for operators of the form

$$\hat{\mathcal{O}}_\pm = A_\pm(y)\frac{d}{dy} + B_\pm(y), \tag{6}$$

where we stress that these operators only depend on the physical variable y, in contrast with previous realizations, where an auxiliary nonphysical variable has to be introduced [17]. In [33], the set of operators (6) is established by means of the integral representation of the confluent hypergeometric function, which, however, turns out not to be valid for the parameters corresponding to the associated Laguerre functions in (2). The integral representation of $M(a, b, z)$ is valid only for $\Re\, b > \Re\, a > 0$, a condition that is not satisfied by the Morse solution $M(-n, 2s+1, y)$ [36]. To avoid this problem we shall deal only with relations among the associated Laguerre functions.

To this end we start by establishing the action of the differential operator d/dy on the Morse functions:

$$\frac{d}{dy}\Psi_n^\nu(y) = -\frac{1}{2}\Psi_n^\nu(y) + \frac{1}{y}s\Psi_n^\nu(y) + N_n^\nu e^{-y/2}y^s\frac{d}{dy}L_n^{2s}(y). \tag{7}$$

One possible relation for the derivative of the associated Laguerre functions is given by [37]:

$$\frac{d}{dy}L_n^\alpha(y) = -\frac{1}{(\alpha+1)}\left[yL_{n-1}^{\alpha+2}(y) + nL_n^\alpha(y)\right]. \tag{8}$$

The substitution of this expression into (7) gives rise to the following relation between the Morse functions belonging to the same potential:

$$\left[\frac{d}{dy}(2s+1) - \left(\frac{1}{y}s - \frac{1}{2}\right)(2s+1) + n\right]\Psi_n^\nu(y) = -\frac{N_n^\nu}{N_{n-1}^\nu}\Psi_{n-1}^\nu(y), \tag{9}$$

from which we can define the operator

$$\hat{K}_- = -\left[\frac{d}{dy}(2s+1) - \frac{1}{y}s(2s+1) + \frac{\nu}{2}\right]\sqrt{\frac{s+1}{s}} \tag{10}$$

with the following effect over the wave functions:

$$\hat{K}_-\Psi_n^\nu(y) = k_-\Psi_{n-1}^\nu(y), \tag{11}$$

where

$$k_- = \sqrt{n(\nu - n)}. \tag{12}$$

As we can see, this operator annihilates the ground state $\Psi_0^\nu(y)$, as expected from a stepdown operator. In Eq. (10) the variable s is to be understood as a diagonal operator depending on n, according to $2s = \nu - 2n - 1$. Note also that the order of the different terms in (10) is important, as these operators do not commute.

We now proceed to find the corresponding creation operator. First we should keep in mind that we need to obtain a relation between $(d/dy)L_n^\alpha(y)$ and $L_{n+1}^{\alpha-2}(y)$, since this implies a relation between $(d/dy)\Psi_n^\nu(y)$ and the Morse function $\Psi_{n-1}^\nu(y)$. To achieve this task we start with the relation

$$y\frac{d}{dy}L_n^\alpha(y) = nL_n^\alpha(y) - (n+\alpha)L_{n-1}^\alpha(y), \tag{13}$$

which, when taking into account that [37]

$$(n+1)L_{n+1}^\alpha(y) - (2n+\alpha+1-y)L_n^\alpha(y) + (n+\alpha)L_{n-1}^\alpha(y) = 0 \tag{14}$$

can be transformed into

$$y\frac{d}{dy}L_n^\alpha(y) = (-n-\alpha-1+y)L_n^\alpha(y) + (n+1)L_{n+1}^\alpha(y). \tag{15}$$

On the other hand, the relation

$$L_n^{\alpha-1}(y) = L_n^\alpha(y) - L_{n-1}^\alpha(y), \tag{16}$$

together with Eq. (14) allows to set up the result

$$\frac{\alpha-1}{n+\alpha}L_{n+1}^\alpha(y) = \left(\frac{\alpha+y-1}{\alpha+n}\right)L_n^\alpha(y) + L_{n+1}^{\alpha-2}(y), \tag{17}$$

which in turn can be substituted into Eq. (15) to give

$$(\alpha-1)\frac{d}{dy}L_n^\alpha(y) = \left[(\alpha+n) - \frac{\alpha(\alpha-1)}{y}\right]L_n^\alpha(y) + \frac{(n+1)(n+\alpha)}{y}L_{n+1}^{\alpha-2}(y). \tag{18}$$

Finally, when this equation is substituted into (7), we obtain

$$\frac{d}{dy}\Psi_n^\nu(y) = \left(-\frac{1}{2} - \frac{s}{y} + \frac{2s+n}{2s-1}\right)\Psi_n^\nu(y) + \frac{N_n^\nu}{N_{n+1}^\nu}\frac{(n+1)(n+2s)}{2s-1}\Psi_{n+1}^\nu(y), \tag{19}$$

which allows to define the creation operator as

$$\hat{K}_+ = \left[\frac{d}{dy}(2s-1) + \frac{1}{y}s(2s-1) - \frac{\nu}{2}\right]\sqrt{\frac{s-1}{s}} \tag{20}$$

satisfying the equation

$$\hat{K}_+\Psi_n^\nu(y) = k_+\Psi_{n+1}^\nu(y), \tag{21}$$

with

$$k_+ = \sqrt{(n+1)(\nu-n-1)}. \tag{22}$$

From Eqs. (9) and (19) the importance of using the correct normalization factors is clear, which was not the case in [33]. Since $\hat{K}_+$ is a raising operator, it is expected to annihilate the last bounded state. Indeed, for such a state $s = 1$ and the square root in (20) makes the operator vanish.

We now study the algebra associated to the operators $\hat{K}_+$ and $\hat{K}_-$. Based on results (11) and (21) we can calculate the commutator $[\hat{K}_+, \hat{K}_-]$:

$$[\hat{K}_+, \hat{K}_-]\Psi_n^\nu(y) = 2k_0\Psi_n^\nu(y), \tag{23}$$

where we have introduced the eigenvalue

$$k_0 = n - \frac{\nu-1}{2}. \tag{24}$$

We can thus define the operator

$$\hat{K}_0 = \hat{n} - \frac{\nu-1}{2}. \tag{25}$$

This operator can be rewritten in terms of differential operators with the help of the differential equation for the Morse functions [38]:

$$\left(y\frac{d^2}{dy^2} + \frac{d}{dy} - \frac{s^2}{y} - \frac{y}{4} + \frac{\nu}{2}\right)\Psi_n^\nu(y) = 0, \tag{26}$$

from which we can establish the identity

$$\hat{K}_0 = \left(y\frac{d^2}{dy^2} + \frac{d}{dy} - \frac{s^2}{y} - \frac{y}{4} + n + \frac{1}{2}\right). \tag{27}$$

Thus the operators $\hat{K}_\pm$ and $\hat{K}_0$ satisfy the commutation relations

$$\begin{aligned} &[\hat{K}_+, \hat{K}_-] = 2\hat{K}_0, \qquad [\hat{K}_0, \hat{K}_-] = -\hat{K}_-, \\ &[\hat{K}_0, \hat{K}_+] = \hat{K}_+, \end{aligned} \tag{28}$$

which correspond to the SU(2) group for the Morse potential. As mentioned earlier, this result is consistent with the description of a finite discrete spectrum and in accordance with previous algebraic descriptions of the bound states of the Morse potential [30, 31]. The operators $\hat{K}_\pm$ and $\hat{K}_0$ are thus equivalent to $\hat{J}_\mp$ and $\hat{J}_0$ used in [30, 31], respectively, where the number of bosons N introduced there is related to ν through $N = \nu - 1$, as we deduce from the Casimir operator:

$$\begin{aligned} \hat{C}\Psi_n^\nu(y) &= \left[\hat{K}_0^2 + \tfrac{1}{2}(\hat{K}_+\hat{K}_- + \hat{K}_-\hat{K}_+)\right]\Psi_n^\nu(y) \\ &= j(j+1)\Psi_n^\nu(y), \end{aligned} \tag{29}$$

where j, the label of the irreducible representations of SU(2), is given by

$$j = \frac{\nu-1}{2} = \frac{N}{2}. \tag{30}$$

From the commutation relations (28) we know that $\hat{K}_0$ is the projection of the angular momentum m, and consequently

$$n - \frac{\nu-1}{2} = m. \tag{31}$$

Therefore the ground state corresponds to $m = j$, while the maximum number of states $n_{\max} = (\nu - 3)/2$ and consequently $m_{\max}(n_{\max}) = -1$. The Morse wave functions are then associated to one branch (in this case to $m \leq -1$) of the SU(2) representations, as expected in [24, 26]. Finally, we should notice that in terms of the SU(2) algebra the Hamiltonian acquires the simple form

$$\hat{H} = -\frac{\hbar\omega}{\nu}\hat{K}_0^2, \tag{32}$$

where

$$\omega = \frac{\hbar\beta^2\nu}{2\mu}. \tag{33}$$

For the wave functions

$$\Psi_n^\nu(y) = \mathcal{N}_n^\nu\hat{K}_+^n\Psi_0^\nu(y), \tag{34}$$

where the normalization constant is obtained through the commutation relations (28), and turns out to be

$$\mathcal{N}_n^\nu = \sqrt{\frac{(\nu-n-1)!}{n!(\nu-1)!}}. \tag{35}$$

For further calculations one can obtain the following expressions in terms of the raising and lowering operators $\hat{K}_\pm$ and $\hat{K}_0$ as

$$\begin{aligned} \frac{d}{dy} &= \hat{K}_+\left[\frac{1}{2(2s-1)}\sqrt{\frac{s}{s-1}}\right] \\ &\quad - \hat{K}_-\left[\frac{1}{2(2s+1)}\sqrt{\frac{s}{s+1}}\right] + \frac{\nu}{2(2s+1)(2s-1)}, \end{aligned} \tag{36}$$

and

$$\begin{aligned} \frac{1}{y} &= \hat{K}_+\left[\frac{1}{2s(2s-1)}\sqrt{\frac{s}{s-1}}\right] \\ &\quad + \hat{K}_-\left[\frac{1}{2s(2s+1)}\sqrt{\frac{s}{s+1}}\right] + \frac{\nu}{(2s+1)(2s-1)}. \end{aligned} \tag{37}$$

The matrix elements of these two functions can be analytically obtained in terms of Eqs. (10) and (20) as

$$\begin{aligned}\left\langle m\left|\frac{1}{y}\right|n\right\rangle &= \frac{1}{\nu-2n-2}\sqrt{\frac{(n+1)(\nu-n-1)}{(\nu-2n-1)(\nu-2n-3)}}\,\delta_{m,n+1}\\ &\quad+\frac{1}{\nu-2n}\sqrt{\frac{n(\nu-n)}{(\nu-2n-1)(\nu-2n+1)}}\,\delta_{m,n-1}\\ &\quad+\frac{\nu}{(\nu-2n-2)(\nu-2n)}\,\delta_{m,n},\end{aligned} \tag{38}$$

$$\begin{aligned}\left\langle m\left|\frac{d}{dy}\right|n\right\rangle &= \frac{1}{2(\nu-2n-2)}\\ &\quad\times\sqrt{\frac{(n+1)(\nu-n-1)(\nu-2n-1)}{\nu-2n-3}}\,\delta_{m,n+1}\\ &\quad-\frac{1}{2(\nu-2n)}\sqrt{\frac{n(\nu-n)(\nu-2n-1)}{\nu-2n+1}}\,\delta_{m,n-1}\\ &\quad+\frac{\nu}{2(\nu-2n)(\nu-2n-2)}\,\delta_{m,n},\end{aligned} \tag{39}$$

which coincide with previous results.

Harmonic Limit

In this section we turn our attention to the harmonic limit in which the Morse potential approaches a harmonic oscillator potential. In this limit $\beta \to 0$ and $V_0 \to \infty$, but keeping the product $k = 2\beta^2 V_0$ finite, so that the expansion of the exponential functions in (1), leads to the harmonic limit

$$\lim_{V_0\to\infty} V_{\mathrm{Morse}} = \tfrac{1}{2}kx^2. \tag{40}$$

We now proceed to analyze the contraction of the SU(2) algebra:

$$G_{\mathrm{SU(2)}} = \{\hat{K}_+, \hat{K}_-, \hat{K}_0\} \tag{41}$$

for this limit. We first note that according to the relation $2s = \nu - 2n - 1$, we have

$$\lim_{\nu\to\infty}\frac{2s}{\nu} = \lim_{\nu\to\infty}\sqrt{\frac{s-1}{s}} = \lim_{\nu\to\infty}\sqrt{\frac{s+1}{s}} = 1. \tag{42}$$

If we now expand the exponential function of the variable y keeping in mind that in the harmonic limit $\beta \to 0$, we find the approximation

$$y \simeq \nu(1-\beta x), \qquad \frac{1}{y} \simeq \frac{1}{\nu}(1+\beta x), \tag{43}$$

which can be used to obtain the corresponding approximation for the derivative

$$\frac{d}{dy} = -\frac{1}{\beta}\frac{1}{y}\frac{d}{dx}, \tag{44}$$

whose harmonic limit turns out to be

$$\lim_{\nu\to\infty}\frac{d}{dy} = \lim_{\nu\to\infty}\left[-\frac{1}{\beta}\frac{1}{\nu}(1+\beta x)\frac{d}{dx}\right] = -\frac{1}{\beta\nu}\frac{d}{dx}. \tag{45}$$

We are now ready to study the harmonic limit of the operators (41), but before doing so it is convenient to introduce the renormalization

$$b^\dagger = \frac{\hat{K}_+}{\sqrt{\nu}}; \qquad b = \frac{\hat{K}_-}{\sqrt{\nu}}; \qquad b_0 = \frac{\hat{K}_0}{\nu}, \tag{46}$$

which, when considered in (10) and (20), leads to

$$\begin{aligned}\lim_{\nu\to\infty} b^\dagger &= \frac{\sqrt{\nu}\beta}{2}x - \frac{1}{\beta\sqrt{\nu}}\frac{d}{dx}\\ &= \sqrt{\frac{\mu\omega}{2\hbar}}x - \sqrt{\frac{\hbar}{2\mu\omega}}\frac{d}{dx} = a^\dagger,\end{aligned} \tag{47a}$$

$$\lim_{\nu\to\infty} b = \sqrt{\frac{\mu\omega}{2\hbar}}x + \sqrt{\frac{\hbar}{2\mu\omega}}\frac{d}{dx} = a, \tag{47b}$$

$$\lim_{\nu\to\infty} b_0 = -\frac{1}{2}, \tag{47c}$$

with ω given by (33). The operators $a^\dagger$ and a satisfy the bosonic commutation relations:

$$[a, a^\dagger] = 1, \qquad [a, a] = [a^\dagger, a^\dagger] = 0, \tag{48}$$

as expected. Thus, in the harmonic limit the SU(2) algebra contracts to the Weyl algebra, i.e.,

$$\lim_{\nu\to\infty} G_{\mathrm{SU(2)}} = \{a^\dagger, a, 1\}. \tag{49}$$

Finally, in terms of the operators (46), the Morse wave functions take the simple form

$$\Psi_n^\nu(y) = \sqrt{\frac{\nu^n(\nu-n-1)!}{n!(\nu-1)!}}(b^\dagger)^n\Psi_0^\nu(y), \tag{50}$$

whose harmonic limit is given by

$$\lim_{\nu\to\infty}\Psi_n^\nu(y) = \frac{1}{\sqrt{n!}}(a^\dagger)^n\phi_0(y), \tag{51}$$

where $\phi_0(y)$ is the ground state for the harmonic oscillator.

Before finishing this section, it is interesting to note that operators $\hat{b}$ and $\hat{b}^\dagger$ can be explicitly expressed in terms of the physical coordinate x and its corresponding momentum $\hat{p}$:

$$\hat{b}^{\dagger} = \left[\frac{e^{\beta x}}{\nu}\left(-\frac{i\hat{p}}{\beta\hbar}+s\right)(2s-1)-\frac{\nu}{2}\right]\sqrt{\frac{s-1}{\nu s}}, \quad (52a)$$

$$\hat{b} = \left[\frac{e^{\beta x}}{\nu}\left(\frac{i\hat{p}}{\beta\hbar}+s\right)(2s+1)-\frac{\nu}{2}\right]\sqrt{\frac{s+1}{\nu s}}. \quad (52b)$$

These expressions essentially correspond to the inverse of the expansions obtained in [30] The exact correspondence should be determined, however, since the normalization factor introduced in (46) is not unique. This analysis will be presented in a future publication.

Franck–Condon Factors

It is well known that the intensity of vibronic spectra can be computed in first-order approximation in terms of the Franck–Condon factors. Their calculation, however, is far from being a straightforward task for the Morse wave functions because of the complicated relations between the variables. Different approximate methods to compute the Franck–Condon factors have been proposed [39–42]. In particular we should mention the closed analytic expression obtained by Matsumoto et al. [41], even though it is expressed as a function of double series containing hypergeometric functions of two variables.

On the other hand, Avram and Drăgănescu in [33] proposed to generate the Franck–Condon factors through the ladder operators $\hat{K}_{\pm,0}$. We find, however, that this approach is not valid, even when using the right expressions for the creation and annihilation operators. The authors in [33] proposed a linear relation through matrix A between the operators $\hat{K}'_{\pm,0}$ and $\hat{K}_{\pm,0}$ associated to different potentials (see Eq. (28) in [33]). We notice, however, that matrix A should contain the information of the displacement of the potential, but this is not the case, since A is independent of x_0. In addition, the relation between the variables y and y' is not linear as

$$y' = b_0\nu'(\nu)^{-\beta'/\beta}y^{\beta'/\beta}, \quad (53)$$

and

$$\frac{d}{dy'} = \frac{\beta\nu^{\beta'/\beta}}{b_0\nu'\beta'}y^{1-\beta'/\beta}\frac{d}{dy}, \quad (54)$$

where $y' = b_0\nu' e^{-\beta' x}$ and $y = \nu e^{-\beta x}$ with $b_0 = e^{-\beta' x_0}$. We note that in [33] the notation α is used for the anharmonicity parameter instead of our β.

Since the relation between the variables y' and y is nonlinear, we expect to obtain $\hat{K}'_{\pm,0}$ as an expansion in powers of $\hat{K}_{\pm,0}$. A linear relation can be obtained only for the special case in which $\beta = \beta'$, and $x_0 = 0$, for which the relation is independent of β.

We now discuss this problem for the same restrictive conditions $\beta = \beta'$, and $x_0 = 0$, by using the correct results presented in this work. To this end, we obtain the relation between $\hat{K}_{\pm,0}$ and $\hat{K}_{\pm,0}$ as the set of equations:

$$\begin{aligned}\hat{K}'_{-} &= \hat{K}_{+}\frac{\nu'}{\nu}\sqrt{\frac{s(s'+1)}{s'(s-1)}}\frac{(2s'+1)(s'-s)}{2s(2s-1)} \\ &\quad + \hat{K}_{-}\frac{\nu'}{\nu}\sqrt{\frac{s(s'+1)}{s'(s+1)}}\frac{(2s'+1)(s'+s)}{2s(2s+1)} \\ &\quad + \left[\frac{\nu'(2s'+1)(2s'-1)}{2(2s-1)(2s+1)}-\frac{\nu'}{2}\right]\sqrt{\frac{s'+1}{s'}}, \end{aligned} \quad (55)$$

and

$$\begin{aligned}\hat{K}'_{+} &= \hat{K}_{+}\frac{\nu'}{\nu}\sqrt{\frac{s(s'-1)}{s'(s-1)}}\frac{(2s'-1)(s'+s)}{2s(2s-1)} \\ &\quad + \hat{K}_{-}\frac{\nu'}{\nu}\sqrt{\frac{s(s'-1)}{s'(s+1)}}\frac{(2s'-1)(s'-s)}{2s(2s+1)} \\ &\quad + \left[\frac{\nu'(2s'-1)(2s'+1)}{2(2s-1)(2s+1)}-\frac{\nu'}{2}\right]\sqrt{\frac{s'-1}{s'}}, \end{aligned} \quad (56)$$

which show that the Franck–Condon factors are very complicated even for this special case.

The Franck–Condon factors obtained in [32] are thus not correct from a fundamental point of view. Here we have pointed out that the Franck–Condon factors in Eqs. (55) and (56) correspond to a particular case. A useful, closed analytic derivation for these factors remains an open problem.

Summary and Conclusions

In this work, we have established the raising and lowering operators for the Morse wave functions following the basic ideas proposed by Avram and Drăgănescu [33]. We have derived a realization only in terms of the physical variable y, without the need of introducing an auxiliary variable [17]. We have also shown that the SU(2) group is the appropriate dynamical symmetry for the bound states of the Morse potential, and not the SO(2,1) group. We have used the SU(2) algebra to express the Morse wave functions in terms of the action of the creation operator $\hat{K}_{+}$ on the ground state. The matrix elements of the operators $1/y$ and d/dy have been analytically obtained in terms of the ladder operators $\hat{K}_{\pm}$ and $\hat{K}_{0}$. This method can be generalized to other functions and represents a simple and elegant approach to obtain these matrix elements in comparison with the traditional techniques in configuration space. The harmonic limit has been also analyzed, showing that the SU(2) algebra contracts to the appropriate Weyl algebra in this limit and we have pointed out that it is not possible to generate the Franck–Condon factors as done in [33], in accordance with the nonlinearity relation between the variable y associated to different potentials. Expression (52) can be inverted to obtain the expansion of any operator depending on the coordinate and momentum as a function of the creation and destruction operators, in a similar way to the analysis presented in [30, 31]. Other applications are currently under consideration.

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