Kratzer potential algebraic representation and matrix elements recurrence formulae

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Generalized recurrence relations for the calculation of multipole matrix elements for Kratzer potential wave functions are obtained operationally. These formulas have been determined by using a non-analytical procedure based on the algebraic representation of the Kratzer eigenfunctions along with the usual ladder properties and commutation relations. For that, the creation and annihilation operators are adequately derived by means of an alternative approach to the factorization method and the exact expressions for matrix elements are achieved with the aid of a relationship between the ladder operators associated with the *bra* and the *ket*. The proposed algebraic approach as well as the formulas for the calculation of matrix elements thus derived are quite simple and direct when compared with other alternative expressions already obtained analytically or pseudo-algebraically by means of the hypervirial theorem commutator algebra.

1. Introduction

The Kratzer potential is a useful two particle interaction model that can be solved for the general case of rotation states different from zero. Although it was proposed long ago [1], only recently has it been reconsidered with renewed attention in studies that use Kratzer wave functions as diatomic molecule basis sets [2], in the calculation of Franck–Condon factors [3] and in the evaluation of two center matrix elements [4], among others. With respect to the latter, the expectation values have been obtained analytically using Kratzer wave functions explicitly for a closed formulation, and pseudo-algebraically with the aid of the hypervirial-like theorem commutator algebra via recursion relations which are given in terms of integrals of decreasing order in the variable instead of decreasing order in the *bra* and *ket* as desirable. For that reason, the recurrence formulas already published demand the use of more than a single matrix element to begin the recursion process as well as cumbersome procedures such as the sum rules or Hellman-Feymann theorem in the evaluation of the needed integrals.

As far as we know, the formal algebraic treatment, based on the ladder operators formalism, has not been exploited for Kratzer functions in spite of having proven its usefulness in the calculation of matrix elements for other potential wave functions. Thus, this work is a contribution in which section 2 is devoted to obtaining the algebraic representation of Kratzer functions. The ladder operators to be discussed are of two types: those shifting the principal quantum number and the ones acting on the orbital number, or equivalent. These creation and annihilation operators are found by using an alternative procedure to the usual Infeld and Hull factorization method. In section 3, as a useful application of the raising and lowering operators associated with Kratzer functions, generalized recurrence relations for the calculation of multipole matrix elements are obtained algebraically. These recursion formulas are derived from the relationship between the ladder operators related to the *bra* and *ket*, the usual creation and annihilation properties and commutation relations.

2. Algebraic representation of Kratzer potential wave functions

Essentially, there are three different ways to obtain ladder operators associated with any potential wave function: by means of the factorization method [5], by quantizing classical dynamical variables [6], and by using the algebraic representation of the orthogonal polynomials directly involved [7]. In this section, in order to obtain the creation and annihilation operators for Kratzer potential wave functions that are adequated to the purpose of this work, we will consider an alternative approach [8] to the Infeld and Hull factorization method [5]. The alternative procedure to be used here gives, for a second order differential equation of the type

$$\alpha(x) f_n'' + \beta(x,n) f_n' + \xi(x,n) f_n = 0\,, \tag{1}$$

linear ladder operator solutions

$$\varphi_n^{\pm} = a^{\pm}(x,n) + b^{\pm}(x,n)\frac{d}{dx} \tag{2}$$

according to the properties

$$\varphi_n^{\pm} f_n = f_{n\pm1}\,. \tag{3}$$

In that case, the raising φ_n^+ and the lowering φ_n^- operators are obtained by solving [8]

$$b^{\pm}(x,n) = A^{\pm}\exp\left(\int \frac{1}{2\alpha(x)}\left(\frac{d\alpha(x)}{dx} + \beta^{\pm}(x,n)\right)dx\right) \tag{4}$$

and

$$a^{\pm}(x,n)\left[\alpha(x)\left(\frac{dQ^{\pm}(x,n)}{dx}+(Q^{\pm}(x,n))^2\right)+Q^{\pm}(x,n)\beta(x,n\pm 1)-\xi^{\pm}(x,n)\right]$$
$$=b^{\pm}(x,n)\frac{d\xi(x,n)}{dx}-P^{\pm}(x,n)\big(\alpha(x)Q^{\pm}(x,n)+\beta(x,n\pm 1)\big)$$
$$-\alpha(x)\frac{dP^{\pm}(x,n)}{dx}, \quad (5)$$

where

$$Q^{\pm}(x,n)=\frac{\beta^{\pm}(x,n)}{2\alpha(x)} \quad (6)$$

and

$$P^{\pm}(x,n)=-\frac{1}{2}\frac{d^2b^{\pm}(x,n)}{dx^2}+\frac{b^{\pm}(x,n)}{2\alpha(x)}\left(\frac{d\beta(x,n)}{dx}+\xi^{\pm}(x,n)\right)$$
$$-\frac{\beta(x,n\pm 1)}{2\alpha(x)}\frac{db^{\pm}(x,n)}{dx} \quad (7)$$

with $\beta^{\pm}(x,n)=\beta(x,n)-\beta(x,n\pm 1)$ and $\xi^{\pm}(x,n)=\xi(x,n)-\xi(x,n\pm 1)$. This method lets us obtain ladder operators of various classes, for example, those acting on the principal and orbital quantum numbers separately depending on the choice of eq. (1) as will be seen next.

2.1. LADDER OPERATORS SHIFTING ν

We will consider the algebraic representation of the Kratzer wave functions using the procedure specified in the above paragraph by assuming $A^{\pm}=\mp 1$ hereafter.

According to Flügge [9] the Schrödinger equation for the radial part of the Kratzer potential is given by

$$\hat{K}_{\nu,\lambda}R_{\nu,\lambda}(x)=0, \quad (8)$$

where

$$\hat{K}_{\nu,\lambda}=\frac{d^2}{dx^2}+\frac{2\gamma^2}{x}-\sigma^2-\frac{\lambda(\lambda-1)}{x^2} \quad (9)$$

with $\sigma^2=\frac{\gamma^4}{(\nu+\lambda)^2}$, $x=\frac{r}{a}$ and $\lambda(\lambda-1)=\gamma^2+l(l+1)$ with $\gamma^2=\frac{2ma^2}{\hbar^2}D$. Thus, in order to obtain the corresponding $\varphi_{\nu}^{\pm}$ creation and annihilation operators associated with Kratzer wave functions, eq. (8) is transformed to

$$z^2\frac{d^2R_{\nu,\lambda}(z)}{dz^2}+\left(z(\nu+\lambda)-\frac{z^2}{4}-\lambda(\lambda-1)\right)R_{\nu,\lambda}(z)=0, \quad (10)$$

where $z = \frac{2\gamma^2}{(\nu+\lambda)}x$. In that case, $\beta^{\pm}(z,\nu) = 0$ and $\xi^{\pm}(z,\nu) = \mp z$ for which $Q^{\pm}(z,\nu) = 0$ and $P^{\pm}(z,\nu) = 1/2$. As a consequence, eq. (4) and eq. (5) are solved to obtain $b^{\pm}(z,\nu) = \mp z$ and $a^{\pm}(z,\nu) = -(\nu+\lambda) + z/2$. That is, according to eq. (2), the $\varphi_\nu^{\pm}$ ladder operators are then given by

$$\varphi_\nu^{\pm} = -(\nu+\lambda) + \frac{z}{2} \mp z\frac{d}{dz} \tag{11}$$

with properties

$$\varphi_\nu^{\pm} R_{\nu,\lambda}(z) = \rho_\nu^{\pm} R_{\nu\pm1,\lambda}(z)\,, \tag{12}$$

where $\rho_\nu^{\pm}$ is related to the normalization constant of the Kratzer wave function for which it is obtained from the latter. That is, given the normalized wave function

$$R_{\nu,\lambda}(z) = C_{\nu,\lambda} z^{\lambda} e^{-z/2} M(-\nu, 2\lambda; z)\,, \tag{13}$$

where

$$C_{\nu,\lambda} = \frac{1}{(2\lambda-1)!}\left[\frac{(\nu+2\lambda-1)!}{2\nu!(\nu+\lambda)}\right]^{1/2}$$

is the corresponding dimensionless normalization constant and $M(a, b; r)$ is the usual confluent hypergeometric function [10], the ladder operators of eq. (11) applied to the above relation yields

$$\varphi_\nu^{\pm} R_{\nu,\lambda}(z) = C_{\nu,\lambda} z^{\lambda} e^{-\frac{z}{2}} \omega_\nu^{\pm} M(-\nu, 2\lambda; z)\,, \tag{14}$$

where

$$\omega_\nu^{\pm} = -\nu + \tfrac{1}{2}(z \pm z) - (\lambda \pm \lambda) \mp z\frac{d}{dz}\,. \tag{15}$$

At this point, it is interesting to note that due to the properties

$$\omega_\nu^{\pm} M(-\nu, 2\lambda; z) = -(\nu+\lambda\pm\lambda) M(-(\nu\pm1), 2\lambda; z)\,, \tag{16}$$

the operators $\omega_\nu^{\pm}$ can be interpreted as the creation and annihilation operators for the confluent hypergeometric function. As a result, by using the above properties in eq. (14) one gets

$$\varphi_\nu^{\pm} R_{\nu,\lambda}(z) = -C_{\nu,\lambda}(\nu+\lambda\pm\lambda) z^{\lambda} e^{-\frac{z}{2}} M(-(\nu\pm1), 2\lambda; z)\,. \tag{17}$$

Thus, the $\rho_\nu^{\pm}$ coefficient in eq. (12) finally becomes

$$\rho_\nu^{\pm} = -\frac{C_{\nu,\lambda}}{C_{\nu\pm1,\lambda}}(\nu+\lambda\pm\lambda)\,. \tag{18}$$

2.2. LADDER OPERATORS ACTING ON λ

Although the linear $\varphi_\lambda^{\pm}$ ladder operators for the λ number can be straightforwardly obtained by using factorization type F in eq. (9), in this section we will follow an alternative approach already mentioned. That is, according to eq. (8) and eq. (9) the Kratzer potential equation is rewritten as

$$\frac{d^2R_{\nu,\lambda+1}(z)}{dz^2}+\left(\frac{\gamma^2}{\sigma}\frac{1}{z}-\frac{1}{4}-\frac{\lambda(\lambda+1)}{z^2}\right)R_{\nu,\lambda+1}(z)=0\,, \tag{19}$$

where we have used a shifting in λ. In that case $\beta^{\pm}(z,\lambda)=0$ and $\xi^{\pm}(z,\lambda) = \pm\frac{1}{z^2}(2\lambda+1\pm1)$ for which $Q^{\pm}(z,\lambda)=0$ and $P^{\pm}(z,\lambda)=-\frac{1}{2z^2}(2\lambda+1\pm1)$. Thus, by solving eq. (4) and eq. (5) one obtains

$$b^{\pm}(z,\lambda)=\mp1 \quad \text{and} \quad a^{\pm}(z,\lambda)=-\frac{\gamma^2}{2\sigma(\lambda+1/2\pm1/2)}+\frac{\lambda+1/2\pm1/2}{z}\,.$$

Finally, the $\varphi_\lambda^{\pm}$ creation and annihilation operators are given, according to eq. (2), by

$$\varphi_\lambda^{\pm}=-\frac{\gamma^2}{2\sigma(\lambda+1/2\pm1/2)}+\frac{\lambda+1/2\pm1/2}{z}\mp\frac{d}{dz} \tag{20}$$

with properties

$$\varphi_{\lambda-1}^{\pm}R_{\nu,\lambda}(z)=\rho_{\lambda-1}^{\pm}R_{\nu,\lambda\pm1}(z)\,, \tag{21}$$

where

$$\rho_{\lambda-1}^{+}=\frac{C_{\nu,\lambda}}{C_{\nu-1,\lambda+1}}\frac{\nu(\nu+2\lambda)}{(2\lambda+1)}\left(\frac{1}{2\lambda}\right)^2 \quad \text{and} \quad \rho_{\lambda-1}^{-}=\frac{C_{\nu,\lambda}}{C_{\nu+1,\lambda-1}}(2\lambda-1)$$

as previously. Besides, similarly to the case with $\rho_\nu^{\pm}$, in this new situation $\rho_\lambda^{\pm}$ is also related to the ladder properties of the creation and annihilation operators associated with the corresponding confluent hypergeometric function. In fact, the equivalent eq. (14), for the λ case, follows:

$$\varphi_{\lambda-1}^{\pm}R_{\nu,\lambda}(z)=C_{\nu,\lambda}z^{\lambda\pm1}e^{-\frac{z}{2}}\omega_{\lambda-1}^{\pm}M(-\nu,2\lambda;z)\,, \tag{22}$$

where

$$\omega_\lambda^{\pm}=z^{\mp1}\left(-\frac{\gamma^2}{2\sigma(\lambda+1/2\pm1/2)}\pm\frac{1}{2}+\frac{(2\lambda+1)(1/2\mp1/2)}{z}\mp\frac{d}{dz}\right) \tag{23}$$

with properties

$$\omega_{\lambda-1}^{\pm}M(-\nu,2\lambda;z)=\eta_{\lambda-1}^{\pm}M(-\nu\pm1,2(\lambda\pm1);z)\,, \tag{24}$$

where

$$\eta_{\lambda-1}^{+}=\frac{\nu(\nu+2\lambda)}{2\lambda+1}\left(\frac{1}{2\lambda}\right)^2 \quad \text{and} \quad \eta_{\lambda-1}^{-}=2\lambda-1$$

are the corresponding normalization constants. That is,

$$\rho^{\pm}_{\lambda-1} = \frac{C_{\nu,\lambda}}{C_{\nu\mp1,\lambda\pm1}}\eta^{\pm}_{\lambda-1}$$

as expected.

Before considering the algebraic treatment of recurrence relations for the calculation of matrix elements, it is interesting that the above ladder operators factorize the corresponding differential equation. In fact, the raising φ^+_ν and the lowering φ^-_ν operators specified by eq. (11) factorize eq. (10) by means of

$$\left(\varphi^+_{\nu-1}\varphi^-_\nu - \nu(\nu-1+2\lambda)\right)R_{\nu,\lambda}(z) = 0 \tag{25a}$$

and conversely

$$\left(\varphi^-_{\nu+1}\varphi^+_\nu - (\nu+1)(\nu+2\lambda)\right)R_{\nu,\lambda}(z) = 0\,. \tag{25b}$$

It should be noted that, as far as we know, these $\varphi^\pm_\nu$ ladder operators have not been reported in the literature before, in spite of their similarity to the corresponding factorization relations given by Infeld and Hull [5]. In our case, the non-operational factor in eqs. (25) corresponds to the product between the normalization constants, for ν and $\nu\pm1$ in each case of the orthogonal polynomial directly involved in the wave function. For example, from eq. (18) and eq. (25a)

$$\nu(\nu+2\lambda-1) = \left[(\nu-1+2\lambda)\frac{C_{\nu-1,\lambda}}{C_{\nu,\lambda}}\right]\left[\nu\frac{C_{\nu,\lambda}}{C_{\nu-1,\lambda}}\right] = \rho^+_{\nu-1}\rho^-_\nu = \eta^+_{\nu-1}\eta^-_\nu\,, \tag{26}$$

where $-(\nu+\lambda\pm\lambda) = \eta^\pm_\nu$ is related to the ladder properties of creation and annihilation operators of the $M(-\nu,2\lambda;z)$ confluent hypergeometric function as given in eq. (16).

In a similar fashion, the ladder operators acting on λ also factorize its corresponding differential equation by means of

$$\left(\varphi^+_{\lambda-1}\varphi^-_\lambda - \nu(\nu+2\lambda)\left(\frac{1}{2\lambda}\right)^2\right)R_{\nu,\lambda+1}(z) = 0 \tag{27a}$$

and conversely

$$\left(\varphi^-_{\lambda+1}\varphi^+_\lambda - \nu(\nu+2(\lambda+1))\left(\frac{1}{2(\lambda+1)}\right)^2\right)R_{\nu,\lambda+1}(z) = 0\,, \tag{27b}$$

where, for example, $\nu(\nu+2\lambda)(1/2\lambda)^2 = \eta^+_{\lambda-1}\eta^-_\lambda$ similarly to the case of ladder operators acting on ν. In short, if eqs. (25) and eqs. (27) are rewritten as

$$\left(\varphi^\pm_{\kappa\mp1}\varphi^\mp_\kappa - \eta^\pm_{\kappa\mp1}\eta^\mp_\kappa\right)R_\kappa(z) = 0\,, \tag{28}$$

where $\kappa = \nu$ or λ, depending on the case, this latter relation can be interpreted as the following rule: the factorization of a second order differential equation is given by the product of non-normalized ladder operators associated with the potential wave function minus the product of the corresponding normalization constants of the orthogonal polynomial, algebraically given, directly involved in the wave function under consideration. The above statement is useful for finding normalization constants and is much simpler than other procedures already developed for a similar purpose, as for example induction or complicated calculations of expectation values.

3. Matrix element recurrence relations

In this section, the operational representation of Kratzer potential wave functions is used to obtain, algebraically, recurrence relations for the calculation of r^k matrix elements. However, although related integrals such as $r^k(d^s/dr^s)$, d^s/dr^s and others are not considered in this work, these can also be obtained by using a similar treatment.

When ladder operators are used, many kinds of recurrence relations come from them depending on the choice of creation and annihilation operators. Particularly, in this work we are going to consider two different types of recursion formulas: from $\varphi_\nu^\pm$ and $\varphi_\lambda^\pm$. In both cases, in order to simplify the calculations, the corresponding raising and lowering operators are transformed into the x variable. That is, in the first case, ladder operators given by eq. (11) are rewritten as

$$\varphi_\nu^\pm = -(\nu+\lambda) + \sigma x \mp x\frac{d}{dx}\,, \tag{29}$$

where $\sigma = \gamma^2/(\nu+\lambda)$ as previously indicated. In that case, the corresponding ladder properties are then

$$\varphi_\nu^\pm|\nu,\lambda\rangle = \rho_\nu^\pm|\nu\pm 1,\lambda\rangle \tag{30}$$

and

$$\langle\nu',\lambda'|\varphi_{\nu'\mp 1}^\pm = \rho_{\nu'\mp 1}^\pm\langle\nu'\mp 1,\lambda'|\,. \tag{31}$$

Following the procedure displayed in ref. [7], the above properties are used in the commutation relation

$$[\varphi_\nu^\pm, x^k] = \mp k x^k \tag{32}$$

along with the relationship between the ladder operators $\varphi_{\nu'}^\pm$ associated with the *bra* $\langle\nu',\lambda'|$ and $\varphi_\nu^\pm$ related to the *ket* $|\nu,\lambda\rangle$,

$$\varphi_\nu^\pm = \varphi_{\nu'}^\pm + (\nu'+\lambda') - (\nu+\lambda) + x(\sigma-\sigma')\,, \tag{33}$$

where $\sigma' = \gamma^2/(\nu'+\lambda')$, in order to obtain the recurrence relations

$$[k+(\nu'+\lambda')-(\nu+\lambda)]\langle\nu',\lambda'|x^k|\nu-1,\lambda\rangle=\rho^+_{\nu-1}\langle\nu',\lambda'|x^k|\nu,\lambda\rangle$$
$$+(\sigma'-\sigma)\langle\nu',\lambda'|x^{k+1}|\nu-1,\lambda\rangle-\rho^+_{\nu'-1}\langle\nu'-1,\lambda'|x^k|\nu-1,\lambda\rangle \tag{34}$$

and

$$[k+(\nu+\lambda)-(\nu'+\lambda')]\langle\nu'-1,\lambda'|x^k|\nu,\lambda\rangle=\rho^-_{\nu'}\langle\nu',\lambda'|x^k|\nu,\lambda\rangle$$
$$+(\sigma-\sigma')\langle\nu'-1,\lambda'|x^{k+1}|\nu,\lambda\rangle-\rho^-_{\nu}\langle\nu'-1,\lambda'|x^k|\nu-1,\lambda\rangle\,. \tag{35}$$

As will be seen next, these recursion formulas are very useful in obtaining some particular cases. Besides, one can avoid the term x^{k+1} in the above equations by using $x^{k+1}=x^k\cdot x$ and $x^{k+1}=x\cdot x^k$, respectively, where x is given by eq. (29). That is, the twin recursion formulas (34) and (35) then becomes

$$\rho^+_{\nu-1}\left(\frac{\sigma'+\sigma}{2\sigma}\right)\langle\nu',\lambda'|x^k|\nu,\lambda\rangle=\rho^+_{\nu'-1}\langle\nu'-1,\lambda'|x^k|\nu-1,\lambda\rangle$$
$$+\left(k-1+(\nu'+\lambda')-(\nu-1+\lambda)\frac{\sigma'}{\sigma}\right)\langle\nu',\lambda'|x^k|\nu-1,\lambda\rangle$$
$$-\rho^-_{\nu-1}\left(\frac{\sigma'-\sigma}{2\sigma}\right)\langle\nu',\lambda'|x^k|\nu-2,\lambda\rangle \tag{36}$$

and

$$\rho^-_{\nu'}\left(\frac{\sigma+\sigma'}{2\sigma'}\right)\langle\nu',\lambda'|x^k|\nu,\lambda\rangle=\rho^-_{\nu}\langle\nu'-1,\lambda'|x^k|\nu-1,\lambda\rangle$$
$$+\left(k-1+(\nu+\lambda)-(\nu'-1+\lambda')\frac{\sigma}{\sigma'}\right)\langle\nu'-1,\lambda'|x^k|\nu,\lambda\rangle$$
$$-\rho^+_{\nu'-2}\left(\frac{\sigma-\sigma'}{2\sigma'}\right)\langle\nu'-2,\lambda'|x^k|\nu,\lambda\rangle\,. \tag{37}$$

It should be noted that in order to get eqs. (34)–(37) we have used $\varphi^\pm_{\nu\mp1}=\pm1+\varphi^\pm_\nu$ as demanded by the properties of eq. (31).

Let us now consider the recursion formulas for λ. Similarly to the above case, in order to obtain recurrence relations from the creation and annihilation operators shifting λ in $R_{\nu,\lambda\pm1}(x)$, it is necessary to consider its ladder properties

$$\varphi^\pm_\lambda|\nu,\lambda+1\rangle=\rho^\pm_\lambda|\nu,\lambda+1\pm1\rangle \tag{38}$$

and

$$\langle\nu',\lambda'|\varphi^\pm_{\lambda'\mp1}=\rho^\pm_{\lambda'\mp1}\langle\nu',\lambda'\mp1| \tag{39}$$

along with the relationship between $\varphi^\pm_\lambda$ and $\varphi^\pm_{\lambda'}$. That is, using

$$\varphi_\lambda^\pm = \left(\frac{\sigma'}{\sigma}\right)\varphi_{\lambda'}^\pm + \frac{(\lambda-\lambda')}{2\sigma}\left(\frac{1}{x} + \frac{\gamma^2}{(\lambda'+1/2\pm 1/2)(\lambda+1/2\pm 1/2)}\right) \tag{40}$$

in the commutation relation

$$x^{k-1} = \mp\frac{1}{k}(\varphi_\lambda^\pm x^k - x^k\varphi_\lambda^\pm) \tag{41}$$

leads to the recurrence relations

$$\begin{aligned}&\frac{\gamma^2(\lambda-\lambda'-1)}{2\sigma\lambda'(\lambda-1)}\langle\nu',\lambda'|x^k|\nu,\lambda\rangle \\ &\quad = \rho_{\lambda-1}^-\langle\nu',\lambda'|x^k|\nu,\lambda-1\rangle - \frac{\lambda-\lambda'-2\sigma k-1}{2\sigma}\langle\nu',\lambda'|x^{k-1}|\nu,\lambda\rangle \\ &\quad\quad - \left(\frac{\sigma'}{\sigma}\right)\rho_{\lambda'}^-\langle\nu',\lambda'+1|x^k|\nu,\lambda\rangle\end{aligned} \tag{42}$$

and

$$\begin{aligned}&\frac{\gamma^2(\lambda-\lambda'+1)}{2\sigma\lambda(\lambda'-1)}\langle\nu',\lambda'|x^k|\nu,\lambda\rangle \\ &\quad = \rho_{\lambda-1}^+\langle\nu',\lambda'|x^k|\nu,\lambda+1\rangle - \frac{\lambda-\lambda'+2\sigma k+1}{2\sigma}\langle\nu',\lambda'|x^{k-1}|\nu,\lambda\rangle \\ &\quad\quad - \left(\frac{\sigma'}{\sigma}\right)\rho_{\lambda'-2}^+\langle\nu',\lambda'-1|x^k|\nu,\lambda\rangle\,.\end{aligned} \tag{43}$$

Finally, in a similar way to the ν case, in order to eliminate the term x^{k-1} in recursion formulas (42) and (43), there are two alternatives: $x^{k-1} = x^k \cdot x^{-1} = x^{-1}\cdot x^k$ with x^{-1} given in terms of the $\varphi_{\lambda-1}^\pm$ ladder operators. That is, from eq. (20)

$$x^{-1} = \frac{2\sigma}{2\lambda-1}(\varphi_{\lambda-1}^+ + \varphi_{\lambda-1}^-) + \frac{\gamma^2}{\lambda(\lambda-1)} \tag{44}$$

one obtains the twin recurrence relations

$$\begin{aligned}&\left(\frac{\lambda+\lambda'-3-2\sigma k}{2\lambda-3}\right)\rho_{\lambda-2}^+\langle\nu',\lambda'|x^k|\nu,\lambda\rangle \\ &\quad = \left(\frac{\sigma'}{\sigma}\right)\rho_{\lambda'-2}^+\langle\nu',\lambda'-1|x^k|\nu,\lambda-1\rangle + \frac{\gamma^2}{2\sigma(\lambda-1)}\left(\frac{\lambda-\lambda'}{\lambda'-1} + \frac{\lambda-\lambda'+2\sigma k}{\lambda-2}\right) \\ &\quad\quad \times\langle\nu',\lambda'|x^k|\nu,\lambda-1\rangle + \left(\frac{\lambda-\lambda'+2\sigma k}{2\lambda-3}\right)\rho_{\lambda-2}^-\langle\nu',\lambda'|x^k|\nu,\lambda-2\rangle\end{aligned} \tag{45}$$

and

$$-\left(\frac{\lambda+\lambda'-3-2\sigma k}{2\lambda'-3}\right)\rho^-_{\lambda'-1}\langle\nu',\lambda'|x^k|\nu,\lambda\rangle$$
$$=\left(\frac{\sigma}{\sigma'}\right)\rho^-_{\lambda-1}\langle\nu',\lambda'-1|x^k|\nu,\lambda-1\rangle-\frac{\gamma^2}{2\sigma'(\lambda'-1)}\left(\frac{\lambda-\lambda'}{\lambda-1}+\frac{\lambda-\lambda'-2\sigma k}{\lambda'-2}\right)$$
$$\times\langle\nu',\lambda'-1|x^k|\nu,\lambda\rangle-\left(\frac{\lambda-\lambda'-2\sigma k}{2\lambda'-3}\right)\rho^+_{\lambda'-3}\langle\nu',\lambda'-2|x^k|\nu,\lambda\rangle \quad (46)$$

depending on the choice of φ^+_λ or φ^-_λ respectively.

3.1. SOME USEFUL PARTICULAR CASES

It seems at first glance that recursion relations (34) and (35) are not of practical use, because they contain mixed integrals of x^k and x^{k+1}. However, in the particular case of $\sigma=\sigma'$ and $\nu=0$ in eq. (35) one obtains

$$\langle\nu',\lambda'|x^k|0,\lambda\rangle=\frac{(k+\lambda-\lambda'-\nu')}{\rho^-_{\nu'}}\langle\nu'-1,\lambda'|x^k|0,\lambda\rangle \quad (47)$$

and similarly for $\nu'=0$ in eq. (34)

$$\langle 0,\lambda'|x^k|\nu,\lambda\rangle=\frac{(k+\lambda'-\lambda-\nu)}{\rho^+_{\nu-1}}\langle 0,\lambda'|x^k|\nu-1,\lambda\rangle\,, \quad (48)$$

where we have used $\rho^-_\nu=0$ if $\nu=0$ and $\rho^+_{\nu'-1}=0$ for $\nu'=0$, respectively. It is interesting to note that eq. (47) can be also written as

$$\langle\nu',\lambda'|x^k|0,\lambda\rangle=\frac{(a-\nu')(a-(\nu'-1))}{\rho^-_{\nu'}\rho^-_{\nu'-1}}\langle\nu'-2,\lambda'|x^k|0,\lambda\rangle$$
$$=\frac{(a-\nu')(a-(\nu'-1))(a-(\nu'-2))}{\rho^-_{\nu'}\rho^-_{\nu'-1}\rho^-_{\nu'-2}}\langle\nu'-3,\lambda'|x^k|0,\lambda\rangle$$
$$\cdots\cdots\cdots\cdots\cdots\cdots$$
$$\cdots\cdots\cdots\cdots\cdots\cdots$$
$$=\frac{(a-\nu')(a-(\nu'-1))\cdots(a-(\nu'-(j-1)))}{\rho^-_{\nu'}\rho^-_{\nu'-1}\cdots\rho^-_{\nu'-(j-1)}}\langle\nu'-j,\lambda'|x^k|0,\lambda\rangle\,, \quad (49)$$

where $a=k-\lambda'+\lambda$. That is, by doing $j\to\nu'$ in eq. (49), the $\langle\nu',\lambda'|x^k|0,\lambda\rangle$ integral is given in terms of the $\langle 0,\lambda'|x^k|0,\lambda\rangle$ lower matrix element by

$$\langle\nu',\lambda'|x^k|0,\lambda\rangle=\frac{(k+\lambda-\lambda'-1)!}{(k+\lambda-\lambda'-1-\nu')!}\left(\prod_{s=0}^{\nu'-1}\rho^-_{\nu'-s}\right)^{-1}\langle 0,\lambda'|x^k|0,\lambda\rangle\,, \quad (50a)$$

where

$$\prod_{s=0}^{\nu'-1} \rho^{-}_{\nu'-\alpha} = (-1)^{\nu'} \left[\frac{\nu'!\lambda'(\nu'+2\lambda'-1)!}{(\nu'+\lambda')(2\lambda'-1)!}\right]^{1/2} . \tag{50b}$$

Symmetrically, eq. (48) becomes

$$\langle 0,\lambda'|x^k|\nu,\lambda\rangle = \frac{(k+\lambda'-\lambda-1)!}{(k+\lambda'-\lambda-1-\nu)!}\left(\prod_{s=1}^{\nu}\rho^{+}_{\nu-s}\right)^{-1}\langle 0,\lambda'|x^k|0,\lambda\rangle , \tag{51a}$$

where

$$\prod_{s=1}^{\nu} \rho^{+}_{\nu-s} = (-1)^{\nu}\left[\frac{\nu!(\nu+2\lambda-1)!(\nu+\lambda)}{\lambda(2\lambda-1)!}\right]^{1/2} . \tag{51b}$$

In any case, the former matrix element is given by

$$\langle 0,\lambda'|x^k|0,\lambda\rangle = C_{0,\lambda'}C_{0,\lambda}(k+\lambda'+\lambda)!(\sigma'_0+\sigma_0)^{-(k+1+\lambda'+\lambda)}(2\sigma'_0)^{\lambda'}(2\sigma_0)^{\lambda} , \tag{52}$$

where $\sigma'_0 = \frac{\gamma^2}{\lambda'}$ and $\sigma_0 = \frac{\gamma^2}{\lambda}$ for $k+\lambda'+\lambda>0$.

4. Concluding remarks

The purpose of the present work is twofold: to provide the algebraic representation of Kratzer potential wave functions and to give new recurrence relations for the calculation of matrix elements. To achieve the first objective, we have used an alternative procedure to the usual factorization method in order to obtain linear creation and annihilation operators for the Kratzer potential wave functions. Advantageously, the proposed approach permits one to determine two kinds of ladder operators that characterize any potential wave function by means of a single multiplicative factor in the original differential equation when needed. On the other hand, in deduction of matrix elements recursion formulas we have used a single relationship between the ladder operators associated with the *bra* and the *ket*. Such a proposition permits us to obtain useful relationships that only need the lower matrix element to begin the recurrence procedure instead of many matrix elements as reported in equivalent formulas already published. In our case, this is because the proposed operational approach is applied to the eigenfunctions more than to the variable or operator between them as usual. In any case, the results and the algebraic methods followed in this work are quite simple and direct when compared with other procedures and formulas used in literature with similar purposes.

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