Algebraic approach to closed formulation of Kratzer potential integrals

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Received 26 June 1996; revised 19 March 1997

In this work, closed form expressions for the calculation of the Kratzer potential integrals are obtained by means of a procedure based on the algebraic representation of the Kratzer eigenfunctions along with the usual ladder properties and commutation relations. For that, the exact formulae for matrix elements are achieved with the aid of the raising operator applied repeatedly over the *ket* and with the lowering operator acting reiteratively over the *bra* for the symmetric closed form expression. Comparatively, the formulae algebraically obtained in this work are quite similar to the ones derived from usual methods involving the evaluation of integrals. Besides, when considering some particular cases the results show that the closed formulae that comes from the algebraic procedure are an improvement to the closed form expressions already published.

1. Introduction

Among many two particle interaction models, the Kratzer potential [7] by itself constitutes one of the most interesting alternatives because it can be exactly solved for the general case of rotation states different from zero. Recently, this potential has been used in studies that utilize the Kratzer wavefunctions as diatomic molecule basis sets [12] and in the evaluation of pseudo two-center matrix elements for undisplaced potentials. With respect to the latter, the closed form expressions for the calculation of the Kratzer potential integrals have been obtained analytically with the aid of the expansion representation of the Laguerre polynomials directly involved [1]. Thus, such equations contain as particular case overlap integrals that are used in the calculations of the Franck–Condon factors for potentials with different depths, although undisplaced [14].

On the other hand, recently Morales et al. [9], using the algebraic representation of the Kratzer potential, have proposed a set of matrix elements recurrence formulae for the evaluation of the Kratzer potential integrals with which they show the usefulness of ladder operator approaches. However, as far as we know such algebraic representation method has not been used to obtain the corresponding closed formulation of Kratzer matrix elements. For that, the purpose of the present work is to use the creation and annihilation operators associated to the Kratzer potential wavefunctions to obtain alternative closed form expressions for the calculation of multipolar integrals, as will be shown next.

2. Closed formulation of Kratzer potential integrals

The algebraic procedures require the knowledge of ladder operators associated with the potential under study. In this respect, there are several options how to obtain creation and annihilation operators associated with any potential wavefunction, such as the factorization method [5], by quantizing classical dynamical variables [8], by using the algebraic representation of the orthogonal polynomials directly involved [11] and by an alternative approach [10] to the Infeld and Hull procedure. In any case, the raising and lowering operators, shifting ν, for Kratzer potential wavefunctions are given by [9]

$$\varphi_\nu^\pm = -(\nu+\lambda) + \sigma x \mp x\,\frac{\mathrm{d}}{\mathrm{d}x}, \tag{1}$$

where $\sigma = \gamma^2/(\nu+\lambda)$, $\gamma^2 = (2ma^2)/\hbar^2 D$ and the other parameters are defined in [3]. The above ladder operators satisfy the following properties:

$$\varphi_\nu^\pm|\nu,\lambda\rangle = \rho_\nu^\pm|\nu\pm 1,\lambda\rangle, \tag{2}$$

$$\langle\nu',\lambda'|\varphi_{\nu'\mp 1}^\pm = \rho_{\nu'\mp 1}^\pm\langle\nu'\pm 1,\lambda'|, \tag{3}$$

where $\rho_\nu^\pm = -[(\nu+1/2\pm 1/2)(\nu+2\lambda-1/2\pm 1/2)]^{1/2}$, and fulfill the commutation relations

$$\left[\varphi_\nu^\pm, x^k\right] = \mp k x^k. \tag{4}$$

Thus, accordingly with the creation properties of $\varphi_{\nu'}^-$ specified in equation (3) we get

$$\langle 0,\lambda'|\varphi_1^-\varphi_2^-\varphi_3^-\cdots\varphi_{\nu'}^- = \rho_1^-\rho_2^-\rho_3^-\cdots\rho_{\nu'}^-\langle\nu',\lambda'| \tag{5}$$

for which, using the commutation relation of equation (4), the x^k integral can be written as

$$\langle\nu',\lambda'|x^k|\nu,\lambda\rangle = \left(\prod_{i=1}^{\nu'}\rho_i'^-\right)^{-1}\langle 0,\lambda'|\left(\prod_{i=1}^{\nu'-1}\varphi_i'^-\right)x^k\big(k+\varphi_{\nu'}^-\big)|\nu,\lambda\rangle, \tag{6}$$

where

$$\prod_{i=1}^{\nu'}\rho_i'^- = (-1)^{\nu'}\left[\frac{\nu'!\Gamma(\nu'+2\lambda')}{\Gamma(2\lambda')}\right]^{1/2}. \tag{7}$$

At this point, by transposing x^k and $\varphi_i'^-$ repeatedly ν times in above equation one obtains

$$\langle \nu', \lambda' | x^k | \nu, \lambda \rangle = \left(\prod_{i=1}^{\nu'} \rho_i'^- \right)^{-1} \langle 0, \lambda' | x^k \prod_{i=1}^{\nu'} \left(k + \varphi_i'^- \right) | \nu, \lambda \rangle. \tag{8}$$

Also, in order to have in the above equation the appropiate ladder operator acting on the *ket*, we use the identity [9]

$$\varphi_i'^- = \varphi_i^- + (\lambda - \lambda') + (\sigma' - \sigma) x, \tag{9}$$

where $\sigma' = \gamma^2/(\nu' + \lambda')$ to obtain

$$\langle \nu', \lambda' | x^k | \nu, \lambda \rangle = \left(\prod_{i=1}^{\nu'} \rho_i'^- \right)^{-1} \langle 0, \lambda' | x^k \prod_{i=1}^{\nu'} \left(\Upsilon x + \mathfrak{R}_i^- \right) | \nu, \lambda \rangle, \tag{10}$$

where $\Upsilon = \sigma' - \sigma$ and $\mathfrak{R}_i^- = k + \lambda - \lambda' + \varphi_i^-$. That is, due to the fact that the operator $\mathfrak{R}_i^-$ has the properties

$$\mathfrak{R}_i^- \pm a = \mathfrak{R}_{i \mp a}^-, \tag{11}$$

$$\mathfrak{R}_i^- x^k = x^k \mathfrak{R}_{i-k}^- \tag{12}$$

and

$$a \mathfrak{R}_i^- + b \mathfrak{R}_j^- = (a+b) \mathfrak{R}_{\frac{ai+bj}{a+b}}^-, \tag{13}$$

we can write

$$\begin{aligned} \prod_{i=1}^{\nu'} \left(\Upsilon x + \mathfrak{R}_i^- \right) &= \prod_{i=1}^{\nu'-1} \left(\Upsilon x + \mathfrak{R}_i^- \right) \left(\Upsilon x + \mathfrak{R}_{\nu'}^- \right) \\ &= \sum_{\alpha=0}^{\nu'} C_\alpha^{\nu'} (\Upsilon x)^{\nu' - \alpha} \prod_{k=1}^{\alpha} \mathfrak{R}_k^-, \end{aligned} \tag{14}$$

where

$$C_\alpha^{\nu'} = \frac{\nu'!}{\alpha! (\nu' - \alpha)!}$$

are the usual binomial coefficients. It should be noticed that one of the products is eliminated by choosing properly the index. In fact, the following holds:

$$\prod_{i=1}^{0} \left(\Upsilon x + \mathfrak{R}_i^- \right) = 1, \tag{15}$$

for which, with $\alpha = p$, equation (10) becomes

$$\langle\nu',\lambda'|x^k|\nu,\lambda\rangle = \left(\prod_{i=1}^{\nu'}\rho_i'^{-}\right)^{-1}\langle 0,\lambda'|x^k \times \sum_{p=0}^{\nu'} C_p^{\nu'}(\Upsilon x)^{\nu'-p}\prod_{l=1}^{p}\big(k+\lambda-\lambda'-l+\varphi_0^-\big)|\nu,\lambda\rangle. \tag{16}$$

Thus, with the purpose to have a suitable annihilation operator acting on the *ket*, we use Vandermonde's formula [6]

$$\prod_{\mu=1}^{i}(a+b-\mu) = \sum_{j=0}^{i} C_j^j \prod_{\mu=1}^{i-j}(a-i-1+\mu)\prod_{w=1}^{j}(b-1+w) \tag{17}$$

along with the property $\varphi_0^- = \nu+\varphi_\nu^-$ in the operator product of equation (16) in order to get

$$\prod_{l=1}^{p}\big(k+\lambda-\lambda'+\nu-l+\varphi_\nu^-\big) = \sum_{\alpha=0}^{p} C_\alpha^p \prod_{l=1}^{p-\alpha}\big(k+\lambda-\lambda'+\nu-p-1+l\big)\prod_{w=1}^{\alpha}\varphi_{\nu-w+1}^-. \tag{18}$$

On the other hand, according to the properties of φ_ν^- on the *ket*

$$\prod_{w=1}^{\alpha}\varphi_{\nu-w+1}^-|\nu,\lambda\rangle = \prod_{w=0}^{\alpha-1}\varphi_{\nu-w}^-|\nu,\lambda\rangle = \prod_{w=0}^{\alpha-1}\rho_{\nu-w}^-|\nu-\alpha,\lambda\rangle \tag{19}$$

one can write equation (16) as

$$\langle\nu',\lambda'|x^k|\nu,\lambda\rangle = \left(\prod_{i=1}^{\nu'}\rho_i'^{-}\right)^{-1}\sum_{p=0}^{\nu'}\sum_{\alpha=0}^{p} C_p^{\nu'}C_\alpha^p\Upsilon^{\nu'-p}\prod_{l=1}^{p-\alpha}\big(k+\lambda-\lambda'+\nu-p-1+l\big) \times \prod_{w=0}^{\alpha-1}\rho_{\nu-w}^-\langle 0,\lambda'|x^{k+\nu'-p}|\nu-\alpha,\lambda\rangle, \tag{20}$$

where

$$\prod_{w=0}^{\alpha-1}\rho_{\nu-w}^- = (-1)^\alpha\left[\frac{\nu!\Gamma(\nu+2\lambda)}{\Gamma(\nu+2\lambda-\alpha)(\nu-\alpha)!}\right]^{1/2}. \tag{21}$$

In a similar way, instead of equation (5) one can now use

$$\varphi_0^+\varphi_1^+\varphi_2^+\cdots\varphi_{\nu-1}^+|0,\lambda\rangle = \rho_0^+\rho_1^+\rho_2^+\cdots\rho_{\nu-1}^+|\nu,\lambda\rangle \tag{22}$$

in order to get the symmetric relationship

$$\langle \nu', \lambda' | x^k | \nu, \lambda \rangle = \left(\prod_{i=1}^{\nu} \rho_{i-1}^{+} \right)^{-1} \sum_{p=0}^{\nu} \sum_{\alpha=0}^{p} C_p^{\nu} C_{\alpha}^{p} (-\Upsilon)^{\nu-p}$$
$$\times \prod_{l=1}^{p-\alpha} \left(k + \lambda' - \lambda + \nu' - p - 1 + l \right) \prod_{w=0}^{\alpha-1} \rho'^{+}_{\nu'-1-w} \langle \nu' - \alpha, \lambda' | x^{k+\nu-p} | 0, \lambda \rangle, \quad (23)$$

where

$$\prod_{w=0}^{\alpha-1} \rho'^{+}_{\nu'-1-w} = (-1)^{\alpha} \left[\frac{\nu'! \Gamma(\nu' + 2\lambda')}{\Gamma(\nu' + 2\lambda' - \alpha)(\nu' - \alpha)!} \right]^{1/2}. \quad (24)$$

At this point, and without any loss of generality we get, by making $\nu = 0$ in equation (20) and $\nu' = 0$ in equation (23), respectively,

$$\langle \nu', \lambda' | x^k | 0, \lambda \rangle = (-1)^{\nu'} \left(\frac{\Gamma(2\lambda')}{\nu'! \Gamma(\nu' + 2\lambda')} \right)^{1/2} \sum_{p=0}^{\nu'} C_p^{\nu'} (\sigma' - \sigma_0)^{\nu'-p}$$
$$\times \frac{\Gamma(k + \lambda - \lambda')}{\Gamma(k + \lambda - \lambda' - p)} \langle 0, \lambda' | x^{k+\nu'-p} | 0, \lambda \rangle \quad (25)$$

and

$$\langle 0, \lambda' | x^k | \nu, \lambda \rangle = (-1)^{\nu} \left(\frac{\Gamma(2\lambda)}{\nu! \Gamma(\nu + 2\lambda)} \right)^{1/2} \sum_{p=0}^{\nu} C_p^{\nu} (\sigma - \sigma_0')^{\nu-p}$$
$$\times \frac{\Gamma(k + \lambda' - \lambda)}{\Gamma(k + \lambda' - \lambda - p)} \langle 0, \lambda' | x^{k+\nu-p} | 0, \lambda \rangle, \quad (26)$$

where the former matrix element is given by

$$\langle 0, \lambda' | x^k | 0, \lambda \rangle = C_{0,\lambda'} C_{0,\lambda} \Gamma(k + \lambda' + \lambda + 1) \left(\sigma_0' + \sigma_0 \right)^{-(k+1+\lambda'+\lambda)}$$
$$\times \left(2\sigma_0' \right)^{\lambda'+1/2} \left(2\sigma_0 \right)^{\lambda+1/2} \quad (27)$$

with $\sigma_0' = \gamma^2/\lambda'$, $\sigma_0 = \gamma^2/\lambda$ and $C_{0,y} = [\Gamma(2y + 1)]^{-1/2}$, where $y = \lambda'$ or $y = \lambda$.

Finally, by using the above relationships in equation (20) and equation (23) we obtain the generalized closed form expression

$$\langle \nu', \lambda' | x^k | \nu, \lambda \rangle = \frac{1}{\left(\sigma_0' + \sigma_0 \right)^k} \left(\frac{2\sigma_0'}{\sigma_0' + \sigma_0} \right)^{\lambda'+1/2} \left(\frac{2\sigma_0}{\sigma_0' + \sigma_0} \right)^{\lambda+1/2}$$
$$\times \frac{(-1)^{\nu'+\nu}}{(\Gamma(2\lambda' + 1)\Gamma(2\lambda + 1))^{1/2}} \left(\frac{\nu! \Gamma(\nu + 2\lambda) \Gamma(2\lambda') \Gamma(2\lambda)}{\nu'! \Gamma(\nu' + 2\lambda')} \right)^{1/2}$$

$$\times \sum_{p=0}^{\nu'} \sum_{\alpha=0}^{p} \sum_{l=0}^{\nu-\alpha} C_p^{\nu'} C_\alpha^p C_l^{\nu-\alpha} \left(\frac{\sigma' - \sigma}{\sigma_0' + \sigma_0} \right)^{\nu'+\nu-p-\alpha-l}$$
$$\times (-1)^{\nu-\alpha-l} \frac{\Gamma(k+\lambda-\lambda'+\nu-\alpha)}{\Gamma(k+\lambda-\lambda'+\nu-p)} \frac{\Gamma(k+\lambda'+\lambda+\nu'+\nu-p+1-\alpha-l)}{(\nu-\alpha)!\Gamma(\nu+2\lambda-\alpha)}$$
$$\times \frac{\Gamma(k+\lambda'-\lambda+\nu'-p)}{\Gamma(k+\lambda'-\lambda+\nu'-p-l)}. \tag{28}$$

At this point, it should be noticed that the algebraic procedure as well as the closed formula for the calculation of the Kratzer potential matrix elements displayed above is rather complicated. However, the usefulness of the above equations becomes clear when we consider some particular cases as shown next.

3. Useful particular results

In order to compare equation (28) with already published results [1,12,14], we are going to consider briefly the corresponding analytical evaluation of x^k Kratzer potential integrals. In fact, by using the Kratzer wavefunctions

$$R_{\nu,\lambda}(r) = \frac{2\sigma}{r} \chi_{\nu,\lambda}(2\sigma r), \tag{29}$$

where

$$\chi_{\nu,\lambda}(z) = (2\sigma)^{-1/2} C_{\nu,\lambda} \mathrm{e}^{(-z/2)} z^\lambda L_\nu^{2\lambda-1}(z)$$

and

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

one gets

$$\langle \nu', \lambda' | r^k | \nu, \lambda \rangle = (2\sigma')^{\lambda'+1/2} (2\sigma)^{\lambda+1/2} C_{\nu',\lambda'} C_{\nu,\lambda} \times \int_0^\infty \mathrm{e}^{-r(\sigma'+\sigma)} r^{k+\lambda'+\lambda} L_{\nu'}^{2\lambda'-1}(2\sigma' r) L_\nu^{2\lambda-1}(2\sigma r)\, \mathrm{d}r. \tag{30}$$

It is interesting to point out that the integral in the above equation can be straightforwardly calculated if we consider the expansion definition for Laguerre polynomials,

$$L_\nu^\lambda(x) = \frac{\Gamma(\nu+\lambda+1)}{\nu!} \sum_{j=0}^{\nu} \frac{(-1)^j}{\Gamma(\lambda+1+j)} C_j^\nu x^j. \tag{31}$$

That is, we obtain

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

$$\times C_{\nu',\lambda'} C_{\nu,\lambda} \frac{\Gamma(\nu' + 2\lambda')}{\nu'!} \frac{\Gamma(\nu + 2\lambda)}{\nu!}$$
$$\times \sum_{i=0}^{\nu'} \sum_{j=0}^{\nu} C_i^{\nu'} C_j^{\nu} \frac{\Gamma(k + \lambda' + \lambda + 1 + i + j)}{\Gamma(2\lambda' + i)\Gamma(2\lambda + j)} \left(\frac{-2\sigma'}{\sigma' + \sigma}\right)^i \left(\frac{-2\sigma}{\sigma' + \sigma}\right)^j. \qquad (32)$$

Finally, making use of the generalized hypergeometric function [4]

$$F_2(\alpha, \beta, \beta', \gamma, \gamma'; x, y) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{(\alpha)_{i+j}(\beta)_i(\beta')_j}{(\gamma)_i(\gamma')_j i! j!} x^i y^j$$

it can be shown that for $\beta = -\nu$ and $\beta' = -\nu'$ integers, sums in above F_2 are finite for which equation (32) trasforms to

$$\langle \nu', \lambda' | x^k | \nu, \lambda \rangle = \left(\frac{2\sigma'}{\sigma' + \sigma}\right)^{\lambda'+1/2} \left(\frac{2\sigma}{\sigma' + \sigma}\right)^{\lambda+1/2} \frac{C_{\nu',\lambda'} C_{\nu,\lambda}}{(\sigma' + \sigma)^k}$$
$$\times \Gamma(\nu + 2\lambda) \frac{\Gamma(\nu' + 2\lambda')\Gamma(k + \lambda' + \lambda + 1)}{\nu! \nu'! \Gamma(2\lambda')\Gamma(2\lambda)}$$
$$\times F_2\left(k + \lambda' + \lambda + 1, -\nu, -\nu', 2\lambda, 2\lambda'; \frac{2\sigma}{\sigma' + \sigma}, \frac{2\sigma'}{\sigma' + \sigma}\right). \qquad (33)$$

At this point, it is interesting to note that this general expression contains as particular case, for $k = 1$ and $\lambda = \lambda'$, the Tugov's formula [13] for the calculation of dipolar matrix elements

$$\langle \nu', \lambda' | x | \nu, \lambda \rangle = \frac{4^\lambda}{\gamma^4} \frac{\big((\nu + \lambda)(\nu' + \lambda)\big)^{\lambda+2}}{((\nu + \lambda) + (\nu' + \lambda))^{2\lambda+2}} \left(\frac{\Gamma(\nu' + 2\lambda)\Gamma(\nu + 2\lambda)}{\nu! \nu'!}\right)^{1/2}$$
$$\times \frac{\Gamma(2\lambda + 2)}{(\Gamma(2\lambda))^2} F_2\left(2\lambda + 2, -\nu, -\nu', 2\lambda, 2\lambda; \frac{2\sigma}{\sigma' + \sigma}, \frac{2\sigma'}{\sigma' + \sigma}\right), \qquad (34)$$

which was obtained by means of a non operational method based on the use of the internuclear potential Green's functions [2].

With this important application, besides the fact that equation (32) and equation (33) contain only two independent sums, it seems at first glance that these closed formulae derived following the non operational procedure of Bastida et al. [1], Waldenstrom and Naqvi [14], Secrest [12] as well as Bunkin and Tugov [2] is simpler than our proposed relationship, equation (28), obtained by means of an algebraic approach or operational method. However, there are some advantages associated with our procedure and formulae that should be pointed out. For example, the succesfulness of the displayed non operator procedure is conditioned by the fact that both wavefunctions are undisplaced, which means that they can be interpreted as being associated to the same potential and by consequence as one-center matrix elements. On the contrary, the proposed algebraic approach can consider displaced potential wavefunctions which is equivalent to establishing real two-center integrals.

With reference to particular cases, in order to compare the closed form equations that come from different approaches, we are going to consider some matrix elements. For example, the closed form expression for the calculation of all diagonal Kratzer potential integrals is given from the non operator method by

$$\langle \nu, \lambda | x^k | \nu, \lambda \rangle = \left(\frac{1}{2\sigma} \right)^k \frac{\Gamma(\nu + 2\lambda)}{2\nu!(\nu + \lambda)} \times \sum_{i=0}^{\nu} \sum_{j=0}^{\nu} C_i^{\nu} C_j^{\nu} (-1)^{i+j} \frac{\Gamma(k + 2\lambda + 1 + i + j)}{\Gamma(2\lambda + i)\Gamma(2\lambda + j)} \tag{35}$$

while the corresponding one deduced from the algebraic approach is

$$\langle \nu, \lambda | x^k | \nu, \lambda \rangle = \left(\frac{1}{2\sigma_0} \right)^k \frac{\Gamma(2\lambda)\Gamma(k + 2\lambda + 1)}{\Gamma(2\lambda + 1)} \times \sum_{\alpha=0}^{\nu} C_{\alpha}^{\nu} \frac{\Gamma(k + \nu - \alpha)}{\Gamma(k - \nu + \alpha)\Gamma(\nu + 2\lambda - \alpha)(\nu - \alpha)!}. \tag{36}$$

Clearly this last equation is simpler than equation (35) because equation (36) contains only one summation.

Another useful result concerns non diagonal matrix elements when $k = 0$ which give rise, respectively, from the analytical result, to

$$\begin{aligned} \langle \nu', \lambda' | \nu, \lambda \rangle = {} & \left(\frac{2\sigma'}{\sigma' + \sigma} \right)^{\lambda'+1/2} \left(\frac{2\sigma}{\sigma' + \sigma} \right)^{\lambda+1/2} \\ & \times C_{\nu',\lambda'} C_{\nu,\lambda} \frac{\Gamma(\nu' + 2\lambda')}{\nu'!} \frac{\Gamma(\nu + 2\lambda)}{\nu!} \\ & \times \sum_{i=0}^{\nu'} \sum_{j=0}^{\nu} C_i^{\nu'} C_j^{\nu} \frac{\Gamma(\lambda' + \lambda + 1 + i + j)}{\Gamma(2\lambda' + i)\Gamma(2\lambda + j)} \left(\frac{-2\sigma'}{\sigma' + \sigma} \right)^i \left(\frac{-2\sigma}{\sigma' + \sigma} \right)^j, \end{aligned} \tag{37}$$

and from the algebraic approach to

$$\begin{aligned} \langle \nu', \lambda' | \nu, \lambda \rangle = {} & \left(\frac{2\sigma_0'}{\sigma_0' + \sigma_0} \right)^{\lambda'+1/2} \left(\frac{2\sigma_0}{\sigma_0' + \sigma_0} \right)^{\lambda+1/2} \frac{(-1)^{\nu'+\nu}}{(\Gamma(2\lambda' + 1)\Gamma(2\lambda + 1))^{1/2}} \\ & \times \left(\frac{\nu!\Gamma(\nu + 2\lambda)\Gamma(2\lambda')\Gamma(2\lambda)}{\nu'!\Gamma(\nu' + 2\lambda')} \right)^{1/2} \sum_{p=0}^{\nu'} \sum_{\alpha=0}^{p} \sum_{l=0}^{\nu-\alpha} C_p^{\nu'} C_{\alpha}^{p} C_l^{\nu-\alpha} \left(\frac{\sigma' - \sigma}{\sigma_0' + \sigma_0} \right)^{\nu'+\nu-p-\alpha-l} \\ & \times (-1)^{\nu-\alpha-l} \frac{\Gamma(\lambda - \lambda' + \nu - \alpha)}{\Gamma(\lambda - \lambda' + \nu - p)} \frac{\Gamma(\lambda' + \lambda + \nu' + \nu - p + 1 - \alpha - l)}{(\nu - \alpha)!\Gamma(\nu + 2\lambda - \alpha)} \\ & \times \frac{\Gamma(\lambda' - \lambda + \nu' - p)}{\Gamma(\lambda' - \lambda + \nu' - p - l)}, \end{aligned} \tag{38}$$

which are, in principle, not very similar. This makes it difficult to decide which one can be considered as an improvement over the other. However, in this respect it is important to note that equation (38) gives rise straightforwardly to $\langle\nu,\lambda|\nu,\lambda\rangle = 1$ which is the normalization condition between Kratzer wavefunctions, while equation (37) that comes from the non operator method, leads to

$$\langle\nu,\lambda|\nu,\lambda\rangle = \frac{\Gamma(\nu+2\lambda)}{2\nu!(\nu+\lambda)}\sum_{i=0}^{\nu}\sum_{j=0}^{\nu}C_i^{\nu}C_j^{\nu}(-1)^{i+j}\frac{\Gamma(2\lambda+1+i+j)}{\Gamma(2\lambda+i)\Gamma(2\lambda+j)}, \tag{39}$$

from where it is not evident orthogonality. Furthermore, the algebraic approach leads to special cases

$$\begin{aligned}\langle\nu',\lambda'|0,\lambda\rangle = {}&(-1)^{\nu'}\left(\frac{\Gamma(2\lambda')}{\nu'!\Gamma(\nu'+2\lambda')}\right)^{1/2}\frac{\Gamma(\lambda-\lambda')}{(\Gamma(2\lambda'+1)\Gamma(2\lambda+1))^{1/2}}\\ &\times\left(\frac{2\sigma_0'}{\sigma_0'+\sigma_0}\right)^{\lambda'+1/2}\left(\frac{2\sigma_0}{\sigma_0+\sigma_0'}\right)^{\lambda+1/2}\\ &\times\sum_{p=0}^{\nu'}C_p^{\nu'}\left(\frac{\sigma'-\sigma}{\sigma_0'+\sigma_0}\right)^{\nu'-p}\frac{\Gamma(\lambda+\lambda'+1+\nu'-p)}{\Gamma(\lambda-\lambda'-p)}\end{aligned} \tag{40}$$

and

$$\begin{aligned}\langle 0,\lambda'|\nu,\lambda\rangle = {}&(-1)^{\nu}\left(\frac{\Gamma(2\lambda)}{\nu!\Gamma(\nu+2\lambda)}\right)^{1/2}\frac{\Gamma(\lambda'-\lambda)}{(\Gamma(2\lambda+1)\Gamma(2\lambda'+1))^{1/2}}\\ &\times\left(\frac{2\sigma_0}{\sigma_0+\sigma_0'}\right)^{\lambda+1/2}\left(\frac{2\sigma_0'}{\sigma_0'+\sigma_0}\right)^{\lambda'+1/2}\\ &\times\sum_{p=0}^{\nu}C_p^{\nu}\left(\frac{\sigma-\sigma'}{\sigma_0+\sigma_0'}\right)^{\nu-p}\frac{\Gamma(\lambda'+\lambda+1+\nu-p)}{\Gamma(\lambda'-\lambda-p)},\end{aligned} \tag{41}$$

which are equations that can be considered as an improvement to the corresponding formulae

$$\begin{aligned}\langle\nu',\lambda'|0,\lambda\rangle = {}&\left(\frac{2\sigma'}{\sigma'+\sigma_0}\right)^{\lambda'+1/2}\left(\frac{2\sigma_0}{\sigma'+\sigma_0}\right)^{\lambda+1/2}\frac{\Gamma(\nu'+2\lambda')}{\nu'!}C_{\nu',\lambda'}C_{0,\lambda}\\ &\times\sum_{i=0}^{\nu'}C_i^{\nu'}\frac{\Gamma(\lambda+\lambda'+1+i)}{\Gamma(2\lambda'+i)}\left(\frac{-2\sigma'}{\sigma'+\sigma_0}\right)^{i}\end{aligned} \tag{42}$$

and

$$\langle 0,\lambda'|\nu,\lambda\rangle = \left(\frac{2\sigma}{\sigma+\sigma_0'}\right)^{\lambda+1/2}\left(\frac{2\sigma_0'}{\sigma+\sigma_0'}\right)^{\lambda'+1/2}\frac{\Gamma(\nu+2\lambda)}{\nu!}C_{0,\lambda'}C_{\nu,\lambda}$$

$$\times \sum_{i=0}^{\nu} C_i^{\nu} \frac{\Gamma(\lambda' + \lambda + 1 + i)}{\Gamma(2\lambda + i)} \left(\frac{-2\sigma}{\sigma + \sigma_0'} \right)^i, \tag{43}$$

that come from the non-algebraic procedure. In fact, although both sets of above equations lead, as expected, to the same result of lower matrix element

$$\langle 0, \lambda' | 0, \lambda \rangle = \left(\frac{2\sigma_0'}{\sigma_0' + \sigma_0} \right)^{\lambda'+1/2} \left(\frac{2\sigma_0}{\sigma_0' + \sigma_0} \right)^{\lambda+1/2} \frac{\Gamma(\lambda + \lambda' + 1)}{(\Gamma(2\lambda+1)\Gamma(2\lambda'+1))^{1/2}}, \tag{44}$$

however, the particular case of $\lambda = \lambda'$ is given, from the equation derived algebraically, by

$$\langle \nu', \lambda | 0, \lambda \rangle = (-1)^{\nu'} \left(\frac{\Gamma(2\lambda)}{\nu'!\Gamma(\nu' + 2\lambda)} \right)^{1/2} \frac{\Gamma(2\lambda + \nu' + 1)}{\Gamma(2\lambda + 1)} \left(\frac{\sigma' - \sigma_0}{\sigma_0' + \sigma_0} \right)^{\nu'}, \tag{45}$$

$$\langle 0, \lambda | \nu, \lambda \rangle = (-1)^{\nu} \left(\frac{\Gamma(2\lambda)}{\nu!\Gamma(\nu + 2\lambda)} \right)^{1/2} \frac{\Gamma(2\lambda + \nu + 1)}{\Gamma(2\lambda + 1)} \left(\frac{\sigma - \sigma_0'}{\sigma_0' + \sigma_0} \right)^{\nu}, \tag{46}$$

which are equations clearly more compact than the corresponding closed formulae analytically obtained:

$$\langle \nu', \lambda | 0, \lambda \rangle = \left(\frac{4\sigma'\sigma_0}{\sigma' + \sigma_0} \right)^{\lambda+1/2} \left(\frac{\Gamma(\nu' + 2\lambda)}{2(\nu' + \lambda)\nu'!\Gamma(2\lambda + 1)} \right)^{1/2} \times \sum_{i=0}^{\nu'} C_i^{\nu'} \frac{\Gamma(2\lambda + 1 + i)}{\Gamma(2\lambda + i)} \left(\frac{-2\sigma'}{\sigma' + \sigma} \right)^i \tag{47}$$

or its symmetric

$$\langle 0, \lambda | \nu, \lambda \rangle = \left(\frac{4\sigma\sigma_0'}{\sigma + \sigma_0'} \right)^{\lambda+1/2} \left(\frac{\Gamma(\nu + 2\lambda)}{2(\nu + \lambda)\nu!\Gamma(2\lambda + 1)} \right)^{1/2} \times \sum_{i=0}^{\nu} C_i^{\nu} \frac{\Gamma(2\lambda + 1 + i)}{\Gamma(2\lambda + i)} \left(\frac{-2\sigma}{\sigma + \sigma'} \right)^i. \tag{48}$$

In any case, the above set of equations are used in the calculation of particular cases of Franck–Condon factors.

4. Concluding remarks

With the present work we provide new closed formulas for the calculation of Kratzer potential matrix elements derived via an algebraic (ladder operator) approach that leads advantageously to improved equations when compared with the corresponding ones already published. Also, the matrix elements derived using ladder properties of the raising and lowering Kratzer operators contain some useful particular cases such as simplified equations for the calculation of Franck–Condon factors for undisplaced potentials. Thus, the proposed approach can be easily extended to consider algebraic representations of other potential as well as real two-center matrix elements.

Acknowledgements

We are indebted to the referees for pointing out the treatment of Kratzer potential from a non-operational procedure based on the Green's functions which has improved the presentation of our results. This work was supported by CONACYT-México, under Scientific Project Number 5-4840E.

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