

# Exact solutions and coherent states for a generalized potential

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**Abstract** Exact solutions of the vibrational Schrödinger equation for a generalized potential energy function  $V(R) = C_0(R - R_e)^2/[aR + (b - a)R_e]^2$  are obtained. It includes those of Dunham, Ogilvie and Simons–Parr–Finlan potentials as special cases corresponding to  $b = 1$ ,  $a = 0, 1/2, 1$ , respectively. The analytical wave functions derived are useful to test the quality of numerical methods or to perform perturbative or variational calculations for the problems that cannot be solved exactly. Coherent states for generalized potential, which minimize the position–momentum uncertainty relation are also constructed.

**Keywords** Exact solutions · Algebraic method · Generalized potential · Anharmonic oscillator · Coherent states

**Mathematics Subject Classification** 81Q05

## 1 Introduction

Exactly solvable potentials [1–12] play an important role in many areas of physics as they can be used to test the quality of numerical methods or to perform perturbative [13] or variational [14] quantum calculations in the case of problems that cannot be solved exactly. Hence, increasing attention has been given to find the most convenient and accurate representation of the potential energy curves, which yield analytical solutions of the vibrational Schrödinger equation. Among the different types of ana-

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lytic functions, for example Padé approximants or power series expansions, the latter give very accurate curves, which satisfactorily reproduce the real potentials for arbitrary values of interatomic separation. An approximation of the potential energy for diatomic systems is usually given in the form

$$V(r) = c_0 \zeta^2 \left( 1 + \sum_{i=1} c_i \xi^i \right) \quad (1)$$

in which

$$\zeta = \begin{cases} \frac{r-r_e}{r_e} & \text{Dunham} \\ \frac{r-r_e}{r} & \text{SPF} \\ \frac{(r-r_e)}{r+r_e} & \text{Tipping} \\ \frac{2(r-r_e)}{r+r_e} & \text{Ogilvie} \end{cases} \quad (2)$$

are the most popular Dunham [15], Simons–Parr–Finlan (SPF) [16], Tipping [17] and Ogilvie [18] expansions, widely used in theoretical analysis of the IR and MW spectra of diatomic systems. In Eq. (2)  $r_e$  is the interatomic separation  $r$  at the minimum of the potential energy  $V(r)$ , whereas  $c_0$  in (1) stands for the potential depth, related to the dissociation energy of the system. The Schrödinger equation for a diatomic oscillator endowed with the reduced atomic mass  $m$

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + V(r) \right] \psi(r)_v = E_v \psi(r)_v \quad (3)$$

can be exactly solved for the first (second-order) term of the Dunham and SPF series (1), whereas no exact solutions for the Tipping–Ogilvie expansions have been obtained so far. In this case only a parabolic expansion of the second-order term in (1) can be used to generate approximate solutions, in contradistinction to SPF potential, for which the second-order exact solutions were derived already in 1920 by Kratzer [1] and in 1926 by Fues [2].

In recent years, the new power-series expansions for molecular potentials with improved ability to fit the experimental data have been introduced. Especially, worth mentioning are generalized Thakkar [19], Mattera [20], Engelke [21], Surkus [22] potentials expanded in variable

$$\zeta = \begin{cases} \text{sign}(p) \left[ 1 - \left( 1 + \frac{r-r_e}{r_e} \right)^{-p} \right] & \text{Thakkar} \\ \text{sign}(p) \left[ 1 - \left( \frac{1+\beta+\frac{r-r_e}{r_e}}{1+\beta} \right)^{-p} \right] & \text{Engelke} \\ \left[ 1 - \left( 1 + \frac{\gamma(r-r_e)}{pr_e} \right)^{-p} \right] & \text{Mattera} \\ \frac{r^p - r_e^p}{r^p + \mu r_e^p} & \text{Surkus} \end{cases} \quad (4)$$

**Table 1** Limiting forms of the generalized variables (4) and (5) obtained by the constraining linear ( $\beta$ ,  $\gamma$ ,  $\mu$ ,  $a$ ,  $b$ )-parameters and nonlinear  $p$ -parameter to values specified in the table

Potential	Thakkar $p$	Engelke $p$ , $\beta$	Mattera $p$ , $\gamma$	Surkus $p$ , $\mu$	Molski $a$ , $b$
Dunham	−1	−1,0	−1,1	−1,0	0,1
SPF	1	1, 0	1, 1	1, 0	1, 1
Tipping		1, 1	1, 1/2	1, 1	1, 2
Ogilvie					1/2, 1

which include Dunham, SPF and Tipping expansions as the special cases (see Table 1). They represent highly flexible functions, of which the parameters can be determined by fitting the experimental data and taking advantage of analytical or numerical techniques. Unfortunately, they do not provide the second-order exact analytical solutions due to the presence of nonlinear  $p$ -parameter defining variables (4).

In this work, we consider a new form of the potential energy of diatomic systems, in which function (1) is expressed in the coordinate

$$\zeta = \frac{r - r_e}{ar + (b - a)r_e} = \begin{cases} \text{Dunham} & b = 1, a = 0 \\ \text{SPF} & b = 1, a = 1 \\ \text{Ogilvie} & b = 1, a = 1/2 \\ \text{Tipping} & b = 2, a = 1 \end{cases} \quad (5)$$

which for  $b=1$  reduces to the variable recently introduced by Molski [23]. For practical calculations  $b$ -parameter should be constrained to the specified above values, whereas  $a$  is an adjustable parameter, which can be determined by fitting the IR and MW spectral data for diatomic molecules. For example,  $a=1.09255(81)$  for GeS [23],  $a=0.5296(25)$  (BrCl),  $a=0.795(10)$  (NaCl),  $a=0.60765(20)$  ( $N_2$ ),  $a=0.5052(16)$  (GeO) [unpublished results]. The influence of  $a$ -parameter on the shape of the potential curves for aforementioned molecules is demonstrated in Fig. 1.

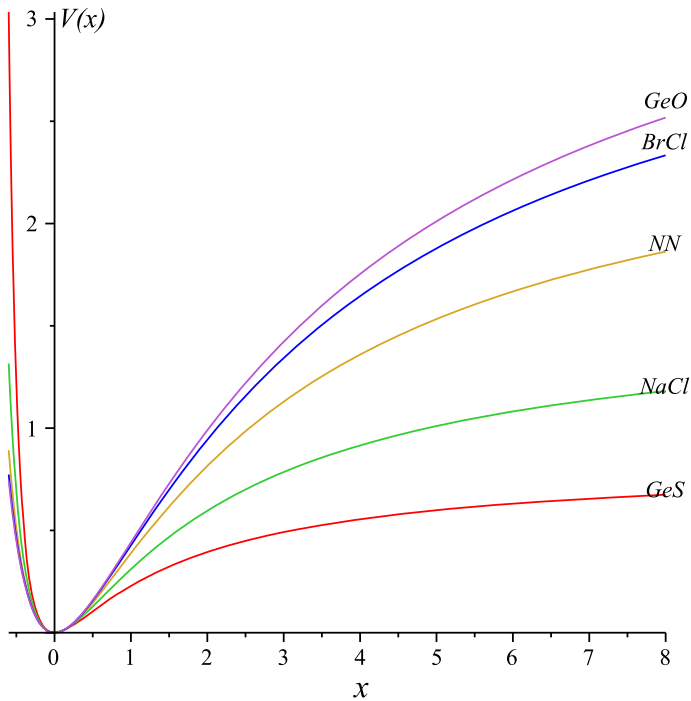
The variable (5) possesses two valuable properties: it remains finite

$$\frac{1}{a - b} \leq \zeta \leq \frac{1}{a} \text{ for } a \neq 0, b \quad (6)$$

throughout the range  $0 < r < \infty$  of molecular existence, and it includes Dunham, SPF, Ogilvie and Tipping coordinates as special cases. It is also noteworthy that the convergence radius

$$R = \frac{2br_e}{1 - a^2} \text{ for } -1 \leq \zeta \leq 1 \quad (7)$$

of the coordinate (5) increases with  $b$  and  $a$  in the range  $|a| < 0, 1 >$ , hence it can be applied for a wide range of interatomic separation  $r$ . The main objective of the present



**Fig. 1** Plots of the generalized potential  $V(x) = c_0[x/(b+ax)]^2$  expressed in Dunham's coordinate  $x = (r - r_e)/r_e$  for  $b = c_0 = 1$  and  $a = 1.09255$  (GeS),  $a = 0.795$  (NaCl),  $a = 0.60765$  ( $N_2$ ),  $a = 0.5296$  (BrCl),  $a = 0.5052$  (GeO) obtained by fitting the IR and MW spectral data [[23], unpublished results]

study is calculating the exact analytical solutions of the Schrödinger equation (3) for the second-order term of the potential (1) expanded in coordinate (5). The approach proposed permits obtaining so far unknown wave functions for the Tipping–Ogilvie oscillator, which emerge as a special case  $(a, b) = [(1/2), 1], (1, 2)$  of the general solutions. The procedure employed in this work is successful as  $(a, b)$ -parameters in (5) are linear, in contradistinction to nonlinear  $p$ -parameter appearing in (4). In the latter case, the exact analytical solutions for potential expansion in variables (4) cannot be determined. The approach proposed also permits constructing the minimum uncertainty coherent states for the oscillator described by the generalized potential as well as by its limiting Tipping–Ogilvie forms.

## 2 Exact analytical solutions

To obtain the exact solutions of the Schrödinger equation

$$\left\{ -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + c_0 \left[ \frac{r - r_e}{ar + (b - a)r_e} \right]^2 \right\} \psi(r)_v = E_v \psi(r)_v \quad (8)$$

we convert it to a new variable

$$y = 1 + \frac{a(r - r_e)}{br_e} \quad (9)$$

transforming original formula into the equation

$$\left\{ -\frac{\hbar^2 a^2}{2mb^2 r_e^2} \frac{d^2}{dy^2} + \frac{c_0}{a^2} \left[ \frac{1-y}{y} \right]^2 \right\} \psi(y)_v = E_v \psi(y)_v \quad (10)$$

amenable to straightforward solution, as Eq. (10) has identical form as wave equation for the Kratzer–Fues [1,2] oscillator expressed in the x-coordinate

$$y(a, b = 1) = \frac{r}{r_e} = x \quad (11)$$

To obtain analytical solutions of Eq. (10), we rewrite it to the form

$$\frac{1}{2} \left\{ -\frac{d^2}{dy^2} + \gamma^2 \left[ \frac{(1-y)^2}{y^2} - 1 \right] + \beta_v^2 \right\} \psi(y)_v = 0 \quad (12)$$

in which

$$\gamma^2 = \frac{2mb^2 r_e^2 c_0}{a^4 \hbar^2} \quad \beta_v^2 = \frac{2mb^2 r_e^2 (c_0/a^2 - E_v)}{a^2 \hbar^2} = \gamma^2 - 2\delta_v^2 \quad (13)$$

Hence, the wave functions and eigenvalues of (12) can be given as [1,2]

$$\psi(y)_v = y^\lambda \exp[-\beta_v y] F(\lambda - \gamma^2/\beta_v, 2\lambda, 2\beta_v y) \quad F(c, b; y) = \sum_{v=0}^{\infty} \frac{\Gamma(c+v)\Gamma(b)y^v}{\Gamma(b+v)\Gamma(c)v!}$$

$$E_v = \frac{c_0}{a^2} \left[ 1 - \frac{\gamma^2}{(v+\lambda)^2} \right] \quad v=0, 1, 2, \dots \quad \lambda = 1/2 + \sqrt{\gamma^2 + 1/4} \quad (14)$$

in which  $F(c, b; y)$  is the confluent hypergeometric function,  $\lambda$  is the positive solution of the parabolic equation  $\lambda^2 - \lambda - \gamma^2 = 0$ , whereas eigenvalues  $E_v$  are derived from the relation

$$\lambda - \frac{\gamma}{\beta_v} = -v \quad (15)$$

for which wave functions (14) converges for  $y \rightarrow \infty$ . Substituting into Eq. (14)  $b=2$ ,  $a=1$  and  $b=1$ ,  $a=1/2$  one gets the unknown solutions of the wave equation for the molecular oscillator described by the second-order term of the Tipping–Ogilvie potential expansion (1).

### 3 Generalized coherent states

The coherent states for harmonic oscillator were discovered by Schrödinger in 1926 [24], and were generalized to include oscillators described by different kinds of anharmonic potentials. Such generalized states are defined in a manner similar to the ordinary coherent states of the harmonic oscillator [25]:

- (i) they are eigenstates of the annihilation operator,
- (ii) they minimize the generalized position–momentum uncertainty relation,
- (iii) they arise from the operation of a unitary displacement operator to the ground state of the oscillator.

It should be pointed out that the definition (iii) relies on the form of the displacement operator, which is specific to the harmonic oscillator [26], hence in this case mainly approximate coherent states can be derived using, for example, Nieto–Simmons [27] or Kais–Levine [28] procedures. The point (ii) defines the so-called *intelligent* coherent states [29]; they not only minimize the Heisenberg uncertainty relation but also maintain this relation in time due to its temporal stability. The coherent states according to the definition (i) are often called Barut–Girardello states [30]. Coherent states of anharmonic oscillators have been constructed using several alternative approaches. In the method proposed by Nieto and Simmons [27], the position and momentum operators are chosen in such a way that the resultant Hamiltonian resembles that for a harmonic oscillator. The coherent states are then determined on condition that they minimize the generalized uncertainty relation in the new variables. Perelomov [31] has derived the coherent states using the irreducible representations of a Lie group. This method has been successfully applied to generate the coherent states of the Morse oscillator [28, 32]. The generalized coherent states can also be constructed using an algebraic method [26], supersymmetric quantum mechanics [33] and mixed supersymmetric–algebraic approach [34]. Applying the above formalisms, the coherent states for Morse [26, 28, 32, 33], generalized Morse [34], Kratzer–Fues [35], Hua Wei [34], Goldman–Krivchenkov [36] and other potentials [34] have been obtained. In this work we focus our attention on the construction of the *intelligent* coherent states for the anharmonic oscillator described by second-order potential (1) expanded in the variable (5). To this aim, we use the factorization method, which decomposes the wave equation (12) into the form [35]

$$\hat{A}^\dagger \hat{A} |v\rangle = (\beta_0^2 - \beta_v^2)/2 |v\rangle \quad |v\rangle = \psi(y)_v \quad (16)$$

including the creation and annihilation operators

$$\hat{A}^\dagger = \frac{1}{\sqrt{2}} \left( -\frac{d}{dy} + \beta_0 - \frac{\lambda}{y} \right) \quad \hat{A} = \frac{1}{\sqrt{2}} \left( \frac{d}{dy} + \beta_0 - \frac{\lambda}{y} \right) \quad (17)$$

Having introduced the operators (17), the coherent states for the generalized potential can be constructed from the ground state solution  $\psi(y)_0$  specified by Eq. (14) for  $v=0$ , yielding eigenstates of the annihilation operator

$$\hat{A}|\alpha\rangle = \alpha|\alpha\rangle \quad |\alpha\rangle = y^\lambda \exp[-\beta_0 y] \exp[\sqrt{2\alpha} y] |0\rangle = \psi(y)_0 \quad (18)$$

Additionally, one may prove that the states (18) minimize the generalized position–momentum uncertainty relation ( $\hbar = 1$ ) [35]

$$\begin{aligned} [\Delta z(y)]^2 [\Delta p]^2 &\geq -\frac{1}{4} \langle \alpha | [z(y), \hat{p}] | \alpha \rangle^2 = \frac{1}{4} \langle \alpha | \frac{\lambda}{y^2} | \alpha \rangle^2 \\ z(y) &= \beta_0 - \frac{\lambda}{y} & \hat{p} &= -i \frac{d}{dy} \end{aligned} \quad (19)$$

The proof is straightforward and needs calculating  $\Delta z(y)$  and  $\Delta p$  appearing in (19) and then demonstrating that  $\Delta z(y) = \Delta p$  [35]

$$\begin{aligned} [\Delta z(y)]^2 &= \langle \alpha | z(y)^2 | \alpha \rangle - \langle \alpha | z(y) | \alpha \rangle^2 = -\frac{1}{2} \langle \alpha | \frac{\lambda}{y^2} | \alpha \rangle \\ [\Delta p]^2 &= \langle \alpha | \hat{p}^2 | \alpha \rangle - \langle \alpha | \hat{p} | \alpha \rangle^2 = -\frac{1}{2} \langle \alpha | \frac{\lambda}{y^2} | \alpha \rangle \end{aligned} \quad (20)$$

The calculations performed reveal that coherent states obtained for the generalized potential are eigenstates of the annihilation operator and minimize the position–momentum uncertainty relation, so they satisfy the two fundamental requirements established for the coherent states of anharmonic oscillators. For  $b=2$ ,  $a=1$  and  $b=1$ ,  $a=1/2$  the derived formula (18) represents the coherent states of the Tipping–Ogilvie oscillator, whereas for  $b=1$ ,  $a=1$  it stands for the coherent states of the Kratzer–Fues oscillator, described by the second-order term of the SPF potential expansion (1).

## 4 Conclusions

The coherent states of anharmonic oscillators make a very useful tool for the investigation of various problems in quantum optics [37], in particular the interactions of molecules with coherent radiation [38], for example, the resonant interactions of the laser beam with molecules producing the coherent effects such as self-induced transparency, soliton formation [39], excitation of a coherent superposition of states [40] and periodic alternations of the refractive index in the molecular systems [40,41]. In the latter case, the variation of the refractive index may appear due to the interaction of the coherent radiation with the coherent rotational [35] and pure vibrational [42] states of the molecules. Investigations in this area require construction of the coherent states for oscillators, described by different types of anharmonic potentials. The generalized potential energy function considered in this work, permits obtaining exact ground-state solution of the vibrational Schrödinger equation, indispensable for creating the coherent states of the generalized oscillator. The proposed new potential expansion seems to be a better representation of the realistic potentials than its special cases proposed by Dunham, Tipping–Ogilvie and Simons–Parr–Finlan. Fitting a-parameter at constrained b-one, we can find the optimal form of the potential expansion for a given molecule at currently available spectral data. In this way, instead of the *rigid*

form of the potential used with constrained  $a$  and  $b$ , one may apply its *flexible* form with  $a$  treated as an additional free-fitted parameter. Its values evaluated for GeS, BrCl, NaCl, N<sub>2</sub> and GeO cover the range  $a = < 0.5052 - 1.09255 >$ , indicating optimal form of the realistic potential energy function for those molecules—for  $b = 1$  it is a combination of Ogilvie and SPF expansions. Exact solutions of the Schrödinger equation obtained for the second-order term of generalized expansion (1) can be employed as basic set of wave functions indispensable in approximate calculations of the energy of diatomic oscillators described by higher-order terms of (1). To this aim variational or perturbational approaches can be used in computation of energy eigenvalues, providing reproduction of the spectral IR and MW data with required accuracy.

### Compliance with ethical standards

**Conflicts of interest** The author of this article has no financial disclosures and conflict of interest.

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