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Generalized and Gaussian coherent states for the Morse potential

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Abstract

In this paper, we consider the one-dimensional anharmonic oscillator, which represents well the anharmonic vibrations in diatomic molecules. For the description of the associate potential we use the Morse potential, which gives a good approximation of the experimentally observed vibrational modes of molecules and hence contributes to the realistic description of the spectrum of diatomic molecules. The generalized and Gaussian coherent states are thus constructed and compared in terms of the localization of the particle in those states. We apply these results to the example of the sodium chloride molecule, $^1\text{H}^{35}\text{Cl}$.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

In quantum mechanics, the one-dimensional harmonic oscillator is described by a quadratic potential. It is a well-known problem and the solution of the corresponding Schrödinger equation can be found in all textbooks on quantum mechanics [1, 2]. It represents a case of an exactly solvable quantum system. However, for most applications in physics, chemistry, biology and material science, a more realistic system is required, such as the anharmonic oscillator, as it describes more accurately, for example, atomic and molecular vibrations [3].

Coherent states have been first introduced as some superposition of energy eigenstates of the quantum harmonic oscillator whose dynamics closely resembles the behaviour of the classic harmonic oscillator. Such definition has been generalized to include other quantum systems with the idea of preserving some of the mathematical and physical properties of the original coherent states [4–8]. The so-called ‘generalized coherent states’ [4] have been constructed

as eigenstates of an annihilation operator [6] both in the case of quantum systems with infinite and finite spectra (see [9] and references therein). On the other hand, the ‘Gaussian coherent states’ [10], defined originally as an approximation of the harmonic oscillator coherent states, have been studied in relation with a good localization with respect to the position of the particle in the case of the square well potential. The generalized and Gaussian coherent states of the same potential have been compared in a recent approach when the energy spectrum may be degenerated [11].

A significant effort has also been made in the last three decades to construct coherent states of general anharmonic potentials [12–14]. On one hand, the interest has been generated by the increasing importance of applications of coherent states to descriptions of physical systems, such as atomic and molecular vibrations, quantum computation and quantum control [15]. On the other hand, the anharmonic potentials, and in particular the Morse potential, represent well the anharmonic behaviour of vibrations in diatomic and complex molecules [13, 16, 17].

In this paper, we consider the one-dimensional anharmonic oscillator, which will be described by using the Morse potential [18]. Indeed, it gives a good approximation of the experimentally observed vibrational modes of molecules and hence contributes to a realistic description of the spectrum of diatomic molecules. In addition, the Morse potential represents a good toy model for studying quantum control [19], as it gives a finite number of bound states (unlike the harmonic oscillator, which gives an infinite number of states) and thus the design of control is limited to a finite regime.

The Morse potential has been studied both in terms of the $SO(2, 1)$ (see, for example [20–25]) and $SU(2)$ groups [26, 27]. The latter description has been exploited in the development of the algebraic model of molecular vibrations in diatomic and polyatomic molecules that incorporates anharmonic effects at the local mode level [26–36], while the former could be relevant for the algebraic determination of the scattering matrices. In $SO(2, 1)$, the Morse Hamiltonian is associated with the Casimir operator in [28–31]. In [24, 25], the Hamiltonians of both, the Morse potential and the modified Pöschl–Teller potential, are obtained and the ladder operators are derived from $SO(2, 1)$. In the case of $SU(2)$, the Morse Hamiltonian is a simple function of the generators [26–32]. The fundamental difference between these two treatments is that $SO(2, 1)$ is a non-compact group which involves either unitary continuous representations or infinite-dimensional discrete representations. Thus, the raising and lowering operators of $SO(2, 1)$ are associated with step variations of the potential depth, keeping a fixed energy [22], while $SU(2)$ formulation involves the description of the bound states which includes only a finite number of states.

In this work, we extend the recent results [11] on generalized and Gaussian coherent states to the case of a quantum system with a finite discrete energy spectrum. We consider different ladder operators and verify some algebra structures or factorization of the Hamiltonian. The definition of generalized coherent states, as some finite superpositions of energy eigenstates, is closely related to the infinite case. We compare the behaviour of these states with the Gaussian ones that are defined independently of any algebra structure. In particular, we show that the generalized and Gaussian coherent states for the Morse potential exhibit a similar behaviour for convenient values of the coherent states parameters. Moreover, such states are minimizing the Heisenberg uncertainty relation in the position and momentum, and they also evolve in time as coherent states.

In section 2, we present the basic concepts of the model. Different sets of the ladder operators are given in section 3. We describe the generalized and Gaussian coherent states of one-dimensional quantum systems in section 4. An application is given with the sodium chloride molecule, $^1\text{H}^{35}\text{Cl}$, in section 5, while conclusions are presented in section 6.

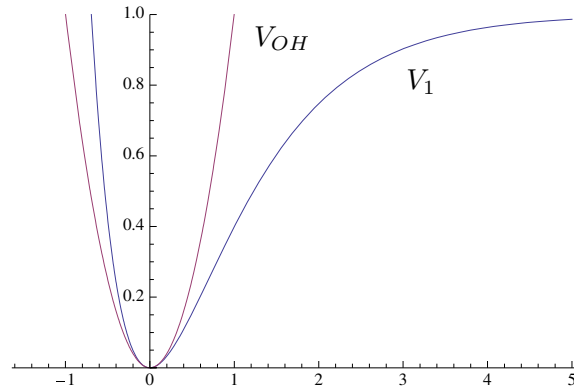


Figure 1. Graphs of V_1 and V_{OH} .

2. The model

The Morse potential in one dimension can be described by a number of equivalent or nearly equivalent forms. In this paper, we shall use the description

$$V_M(x) = V_0(e^{-2\beta x} - 2e^{-\beta x}), \quad (1)$$

where x is the space variable, which in the context of diatomic molecule represents the displacement of the two atoms from their equilibrium positions, V_0 is a scaling energy constant representing the depth of the potential well at equilibrium $x = 0$ and β is the parameter of the model, related to the characteristics of the Morse well, such as its depth and width. Another possible choice of the potential is

$$V_1 = V_0(1 - e^{-\beta x})^2 = V_M + V_0. \quad (2)$$

Let us mention that the harmonic oscillator limit $V_{OH} = \frac{1}{2}kx^2$ is obtained when we consider the potential V_1 with $V_0 = \frac{k}{2\beta^2}$ and take the limit $\beta x \rightarrow 0$. The well-known graphs of V_1 and V_{OH} , with $\frac{k}{\beta^2} = 2$, are shown in figure 1.

Let us consider the one-dimensional quantum oscillator model with the Hamiltonian \mathcal{H} :

$$\mathcal{H}\psi(x) = \left(-\frac{\hbar^2}{2m_r} \frac{d^2}{dx^2} + V_M(x) \right) \psi(x) = E\psi(x), \quad (3)$$

where \hbar is the Plank constant and m_r is the reduced mass of the oscillator composed of two particles of masses m_1 and m_2 ,

$$\frac{1}{m_r} = \frac{1}{m_1} + \frac{1}{m_2}. \quad (4)$$

The first term of (3) gives the kinetic energy and the second term gives the potential energy of the oscillator described by the Morse potential (1).

The eigenvalues and eigenfunctions of this model are well known (see, for example [13]). The energy eigenvalues are

$$E_n = -\frac{\hbar^2}{2m_r} \beta^2 s^2, \quad (5)$$

with

$$s = \epsilon_n = \frac{\nu - 1}{2} - n, \quad (6)$$

and n takes a finite number of values, i.e. $\{n = 0, 1, 2, \dots, n_{\max} - 1\}$, $n_{\max} = [p]$, with $[p]$ the integer part of $p = \frac{\nu-1}{2}$. We thus have

$$E_{n+1} - E_n = \frac{\hbar^2}{2m_r} \beta^2 (\nu - 2(n+1)), \quad (7)$$

showing that consecutive energies are not equally spaced due to the presence of the term depending on n , in contrast to the case of the harmonic oscillator. For later use, we also introduce the difference

$$e(n) = (\epsilon_n^2 - \epsilon_0^2) = -\frac{2m_r}{\hbar^2 \beta^2} (E_n - E_0) = n(n - \nu + 1), \quad (8)$$

which corresponds to shifted energies such that $e(0) = 0$. The energy eigenfunctions, for the discrete spectrum, are given in terms of associated Laguerre functions, denoted by L_n^{2s} , as

$$\psi_n^\nu(x) = \mathcal{N}_n e^{-\frac{\nu}{2}y} y^s L_n^{2s}(y), \quad (9)$$

where \mathcal{N}_n is a normalization factor to be determined. The new variable y is used instead of x and takes the form

$$y = \nu e^{-\beta x}, \quad \nu = \sqrt{\frac{8m_r V_0}{\beta^2 \hbar^2}}. \quad (10)$$

Thus, the constant V_0 can be written as

$$V_0 = \frac{\beta^2 \hbar^2}{2m_r} \left(\frac{\nu}{2}\right)^2. \quad (11)$$

The parameters of the Morse potential can be expressed in terms of the Dunham constants, well known in molecular spectroscopy, the values of which are listed for all diatomic molecules in [3].

In order to get the good normalization factor, we use the orthogonality relation of the associated Laguerre functions which, in terms of the variable y given in (10), is

$$\int_0^\infty L_n^{\nu-1-2n}(y) L_m^{\nu-1-2m}(y) y^{\nu-2-(n+m)} e^{-y} dy = \frac{\Gamma(\nu-n)}{(\nu-1-2n)\Gamma(n+1)} \delta_{nm}. \quad (12)$$

In this relation, we have taken into account the fact that the factor s appearing in the associated Laguerre functions L_n^{2s} is not independent of n .

This leads to the expected orthogonality relation on the energy eigenfunctions $\psi_n^\nu(x)$ depending on the original space variable x :

$$\int_{-\infty}^\infty \psi_n^\nu(x) \psi_m^\nu(x) dx = \delta_{nm}, \quad (13)$$

if the normalization factor \mathcal{N}_n in (9) is chosen as

$$\mathcal{N}_n = \sqrt{\frac{\beta(\nu-2n-1)\Gamma(n+1)}{\Gamma(\nu-n)}}. \quad (14)$$

The normalization is possible for all states, including the last state $n = n_{\max} - 1$.

3. Ladder operators and $SU(2)$

The ladder operators for the Morse potential have been obtained in particular in [13]. Here three different sets of such operators are obtained. Discussions on the construction of such

sets for one general dimensional quantum systems may be found in different recent papers [9, 37–42]. They must all satisfy, at first

$$A^- \psi_n^v = \sqrt{k(n)} \psi_{n-1}^v, \quad A^+ \psi_n^v = \sqrt{k(n+1)} \psi_{n+1}^v, \quad (15)$$

where the quantity $k(n)$ will be chosen, in a second step, to impose additional constraints to the ladder operators. The number operator is defined, as usual, by

$$N \psi_n^v = n \psi_n^v \quad (16)$$

and any function of N thus acts as

$$F(N) \psi_n^v = F(n) \psi_n^v. \quad (17)$$

The energy eigenvalue equation for the Morse potential, written in terms of the variable $y = v e^{-\beta x}$, leads to useful relations between the eigenstates that include $\psi_{n-1}^v, \psi_n^v, \psi_{n+1}^v$. We start with the following ‘annihilation’ and ‘creation’ relations [13]:

$$-(v-2n) \frac{d}{dy} \psi_n^v + \frac{(v-2n-1)(v-2n)}{2y} \psi_n^v - \frac{v}{2} \psi_n^v = \sqrt{\frac{v-2n-1}{v-2n+1}} (\sqrt{k^v(n)} \psi_{n-1}^v), \quad (18)$$

$$(v-2n-2) \frac{d}{dy} \psi_n^v + \frac{(v-2n-1)(v-2n-2)}{2y} \psi_n^v - \frac{v}{2} \psi_n^v = \sqrt{\frac{v-2n-1}{v-2n-3}} (\sqrt{k^v(n+1)} \psi_{n+1}^v), \quad (19)$$

where

$$k^v(n) = n(v-n). \quad (20)$$

These relations are both valid with $n \in [0, n_{\max} - 1]$.

We can now choose the following ladder operators, which are differential operators in the variable y and are also expressed in terms of the operator N defined by equation (16). The different choices correspond to additional properties which will be specified in each case.

(1) $su(2)$ -type ladder operators [13]: they are given by

$$K_- = - \left[\frac{d}{dy} (v-2N) - \frac{(v-2N-1)(v-2N)}{2y} + \frac{v}{2} \right] \sqrt{\frac{v-2N+1}{v-2N-1}}, \quad (21)$$

$$K_+ = \left[\frac{d}{dy} (v-2N-2) + \frac{(v-2N-1)(v-2N-2)}{2y} - \frac{v}{2} \right] \sqrt{\frac{v-2N-3}{v-2N-1}}, \quad (22)$$

with

$$K_- \psi_n^v = \sqrt{k^v(n)} \psi_{n-1}^v, \quad K_+ \psi_n^v = \sqrt{k^v(n+1)} \psi_{n+1}^v. \quad (23)$$

Let us recall that these relations are true for $n \in [0, n_{\max} - 1]$.

They satisfy the commutation relations of the $su(2)$ algebra. Indeed, introducing $K_0 = N - \frac{v-1}{2}$, we get

$$[K_+, K_-] = 2K_0. \quad (24)$$

Let us mention that, in terms of the original variable x using (10), we get

$$K_- = \left[\frac{e^{\beta x}}{v\beta} \left(\frac{d}{dx} + \frac{\beta}{2}(v - 2N - 1) \right) (v - 2N) - \frac{v}{2} \right] K(N), \quad (25)$$

$$K_+ = (K(N))^{-1} \left[\frac{e^{\beta x}}{v\beta} \left(-\frac{d}{dx} + \frac{\beta}{2}(v - 2N - 1) \right) (v - 2N - 2) - \frac{v}{2} \right], \quad (26)$$

with

$$K(N) = \sqrt{\frac{v - 2N + 1}{v - 2N - 1}}. \quad (27)$$

It is interesting to mention that our ladder operators for the Morse potential can thus be written in the general form:

$$K_- = F_-(x, N) \frac{d}{dx} + G_-(x, N), \quad (28)$$

$$K_+ = F_+(x, N) \frac{d}{dx} + G_+(x, N). \quad (29)$$

This form will be useful in further work. These expressions, and the following ones, can be compared with the ones obtained in [42].

- (2) Factorization of the Hamiltonian [9]: the ladder operators are constructed in such a way that they satisfy

$$a^- \psi_n^v = \sqrt{e(n)} \psi_{n-1}^v, \quad a^+ \psi_n^v = \sqrt{e(n+1)} \psi_{n+1}^v, \quad n \in [0, n_{\max} - 1], \quad (30)$$

with $e(n)$ given by (8) and

$$\left(\frac{\hbar^2}{2\mu} \beta^2 \right) a^+ a^- = \mathcal{H} - E_0. \quad (31)$$

This means that the shifted Hamiltonian (with fundamental energy equal to zero) is a product of the ladder operators. This relation is valid for all physical states ψ_n^v such that $n \in [0, n_{\max} - 1]$.

Moreover, we get

$$[a^+, a^-] \psi_n^v = (e(n) - e(n+1)) \psi_n^v = -(2K_0 + 1) \psi_n^v, \quad n \in [0, n_{\max} - 1]. \quad (32)$$

It is easy to see that they may be expressed simply in terms of the preceding ones as

$$a^- = K_- A(N), \quad a^+ = A(N) K_+, \quad (33)$$

with

$$A(N) = \sqrt{\frac{N - v + 1}{v - N}}. \quad (34)$$

- (3) Oscillator-like ladder operators [9, 37–42]: they have to satisfy

$$b^- \psi_n^v = \sqrt{n} \psi_{n-1}^v, \quad b^+ \psi_n^v = \sqrt{n+1} \psi_{n+1}^v, \quad (35)$$

so that

$$[b^-, b^+] \psi_n^v = \psi_n^v, \quad n \in [0, n_{\max} - 1]. \quad (36)$$

Again, they are easily connected to the preceding ones:

$$b^- = a^- \sqrt{\frac{1}{N - v + 1}} = K_- \sqrt{\frac{1}{v - N}}, \quad b^+ = \sqrt{\frac{1}{N - v + 1}} a^+ = \sqrt{\frac{1}{v - N}} K_+. \quad (37)$$

4. Generalized and Gaussian coherent states

Coherent states are usually described as a superposition of energy eigenstates of a quantum system with a discrete infinite energy spectrum that satisfy some mathematical and physical properties. They have been introduced originally for the harmonic oscillator because of their property to be ‘quasi-classical’ states. They have been generalized in different ways and for many systems with non-degenerate and degenerate spectra [4, 6, 7, 8, 9, 11, 13, 38, 40].

Here we are interested in the description of those states in two ways. First, we will consider the ‘generalized coherent states’ which can be viewed as eigenstates of an annihilation operator for the case of a quantum system with a discrete infinite energy spectrum. Second, we will give the ‘Gaussian coherent states’ which are defined as being well localized in the position x of the particle.

The example of the Morse potential deals with the particular case of a finite non-degenerate discrete energy spectrum. The definitions of the preceding states will thus be adapted to include a finite superposition of energy eigenstates.

4.1. General context

Let us assume that the system is described by the Hamiltonian H and admits a non-degenerate discrete infinite or finite energy spectrum. The set of energies is thus denoted by $\{E_n, n \in I\}$, where I is \mathbb{N} or a finite interval of \mathbb{N} . We assume the spectrum is in increasing order with respect to n :

$$E_0 < E_1 < E_2 < \cdots < E_{n-1} < E_n < \cdots, \quad n \in I. \quad (38)$$

The corresponding energy eigenstates are, as usual, denoted by $|\psi_n\rangle$. They satisfy the orthogonality relation $\langle \psi_m | \psi_n \rangle = \delta_{mn}$, $\forall n, m \in I$. We also have

$$\mathcal{H}|\psi_n\rangle = E_n|\psi_n\rangle, \quad \forall n \in I. \quad (39)$$

The generalized coherent states have been defined by Klauder [8] (the usual phase factor introduced to assure temporal stability is taken to 1 in our paper to simplify the discussion but would be considered in the future extended work) as

$$|z\rangle = \frac{1}{\sqrt{\mathcal{N}(|z|^2)}} \sum_{n \in I} \frac{z^n}{\sqrt{\rho_n}} |\psi_n\rangle, \quad \text{where } z \in \mathbb{C}. \quad (40)$$

The coherent states are supposed to be normalized, i.e. the positive normalization constant $\mathcal{N}(|z|^2)$ is chosen so that $\langle z | z \rangle = 1$. The quantities ρ_n are a set of strictly positive parameters that will be related to the energy eigenvalues. They correspond to a momentum problem obtained from the resolution of the identity of the coherent states (see [8] for details).

In the case of an infinite energy spectrum for H and if we take the annihilation and creation operators as defined in equation (15), we get [9]

$$\rho_n = k(1)k(2) \cdots k(n), \quad \rho_0 = 1 \quad (41)$$

and the states (40) are eigenstates of A^- . In the case of the harmonic oscillator, let us recall that we have $\rho_n = n!$, i.e. the product of the shifted energies. The states (40) are eigenstates of the usual harmonic oscillator annihilator operator that satisfy (35). They are effectively the original standard ones.

In the case of a finite spectrum, the states defined in (40) with ρ_n given by (41) are not eigenstates of the annihilation operator A^- because in the expression of $A^-|z\rangle$, the last state is missing. We will show that, in practice, the last term on the right hand side does not contribute

significantly to the sum in the coherent states $|z\rangle$. We can thus say that our coherent states are, in the finite case, ‘almost’ eigenstates of the annihilation operator.

Gaussian coherent states [10] have been defined to give a good approximation of the standard coherent states of the harmonic oscillator. They have been generalized in a way that they lead to a good localization with respect to the position of the particle. We take

$$|\mu, \sigma\rangle = \frac{1}{\sqrt{\mathcal{N}(\mu, \sigma)}} \sum_{n \in I} e^{-\frac{(n-\mu)^2}{4\sigma^2}} |\psi_n\rangle, \quad \text{where } \{\mu, \sigma\} \in \mathbb{R}, \quad (42)$$

and

$$\mathcal{N}(\mu, \sigma) = \sum_{n \in I} e^{-\frac{(n-\mu)^2}{2\sigma^2}}. \quad (43)$$

They are clearly defined independently of the existence of an annihilation operator. The real parameters μ and σ will have to be adjusted to get a good localization of the particle. In the following, we want to compare the Gaussian coherent states with the generalized ones and find a good choice for the parameters z and $\{\mu, \sigma\}$.

In the harmonic oscillator case, it has been shown that the Gaussian coherent states are obtained as a good approximation [10, 11] of the generalized ones if we have to take

$$\mu = \langle N \rangle, \quad \sigma = \Delta N = \sqrt{\langle N^2 \rangle - \langle N \rangle^2}, \quad (44)$$

which gives $\langle N \rangle = (\Delta N)^2 = |z|^2$. Such relations (44) could help us for the case of the Morse potential and the associated coherent states.

4.2. Anharmonic oscillator case

In this case, the eigenfunctions are given by $|\psi_n\rangle = \psi_n^v$ which are normalized with respect to the inner product given in (13). Generalized coherent states may be constructed using equation (40) so that we get

$$\Psi^v(z, x) = \frac{1}{\sqrt{\mathcal{N}_0^v(|z|^2)}} \sum_{n=0}^{n_{\max}-1} \frac{z^n}{(\rho_n)^{1/2}} \psi_n^v(x). \quad (45)$$

Taking ρ_n as the product of the shifted energies like in the harmonic oscillator case, we get

$$\rho_n = \prod_{k=1}^n (\epsilon_k - \epsilon_0) = n! \frac{\Gamma(v-1)}{\Gamma(v-n-1)} \quad (46)$$

and

$$\mathcal{N}_0^v(|z|^2) = \frac{1}{\Gamma(v-1)} \sum_{n=0}^{n_{\max}-1} \frac{|z|^{2n}}{n!} \Gamma(v-n-1). \quad (47)$$

The final form of the generalized coherent states (45) is thus

$$\Psi^v(z, x) = C_0 \sum_{n=0}^{n_{\max}-1} \left(\frac{\Gamma(v-n-1)}{n!} \right)^{\frac{1}{2}} z^n \psi_n^v(x), \quad (48)$$

where $C_0 = (\Gamma(v-1) \mathcal{N}_0^v(|z|^2))^{-\frac{1}{2}}$.

The reason for such a choice is that these states are ‘almost’ eigenstates of the annihilation operator a^- satisfying (30) which, in the limit $\beta x \rightarrow 0$, will give rise to the harmonic oscillator coherent states [13].

The Gaussian coherent states are obtained directly from (42). We get

$$\Phi^{\nu}(\mu, \sigma, x) = \frac{1}{\sqrt{\mathcal{N}(\mu, \sigma)}} \sum_{n=0}^{n_{\max}-1} e^{-\frac{(n-\mu)^2}{4\sigma^2}} \psi_n^{\nu}(x). \quad (49)$$

We can now compute the density probabilities for the generalized coherent states $\Psi(z, x)$ and the Gaussian ones $\Phi^{\nu}(\mu, \sigma, x)$. In this context, we use the following expressions, which are computed in the coherent states (48):

$$\begin{aligned} \langle N \rangle &= C_0^2 |z|^2 \sum_{n=0}^{n_{\max}-1} \left(\frac{\Gamma(\nu - n - 2)}{n!} \right) |z|^{2n}, \\ \langle N^2 \rangle &= C_0^2 |z|^2 \sum_{n=0}^{n_{\max}-1} \left(\frac{(n+1)\Gamma(\nu - n - 2)}{n!} \right) |z|^{2n} \end{aligned} \quad (50)$$

and

$$\Delta N = \sqrt{\langle N^2 \rangle - \langle N \rangle^2}. \quad (51)$$

They will give the values of the parameters μ and σ , i.e. $\langle N \rangle \approx \mu$ and $\Delta N \approx \sigma$.

If we now consider the time-dependent Schrodinger equation

$$i\hbar \partial_t \psi(x; t) = \mathcal{H} \psi(x; t), \quad (52)$$

with the time dependence of the wavefunction expressed by

$$\psi(x; t) = e^{-\frac{iE}{\hbar}t} \psi(x), \quad (53)$$

we can easily compute the corresponding time evolution for the generalized and Gaussian coherent states. Indeed, we have

$$\Psi^{\nu}(z, x; t) = \frac{1}{\sqrt{\mathcal{N}_0^{\nu}(|z|^2)}} \sum_{n=0}^{n_{\max}-1} \frac{z^n}{(\rho_n)^{1/2}} e^{-\frac{iE_n}{\hbar}t} \psi_n^{\nu}(x) \quad (54)$$

and

$$\Phi^{\nu}(\mu, \sigma, x; t) = \frac{1}{\sqrt{\mathcal{N}(\mu, \sigma)}} \sum_{n=0}^{n_{\max}-1} e^{-\frac{(n-\mu)^2}{4\sigma^2}} e^{-\frac{iE_n}{\hbar}t} \psi_n^{\nu}(x), \quad (55)$$

where E_n is given in (5). An illustration of the behaviour of those states with respect to the time evolution will be given in section 5 and we will show a good localization while the time evolves.

We will also show in the example of section 5 that, for the values of z and μ, σ that give a good localization of the particle, our coherent states approximate very well the least value of the Heisenberg uncertainty relation with respect to the position and momentum operators, i.e.

$$(\Delta x)^2 (\Delta p)^2 \approx \frac{1}{4} \quad (\hbar = 1). \quad (56)$$

5. Applications: coherent states for $^1\text{H}^{35}\text{Cl}$

To illustrate the concepts of generalized and coherent states for diatomic molecules, we consider the molecule of sodium chloride, $^1\text{H}^{35}\text{Cl}$. The value of ν can be calculated from (10), with the values of m_r, β and V_0 published, for example, in [3]. Alternatively, using the well-known consistency conditions between the Morse parameters V_0 and β and the Dunham coefficients [3], one can show that [36]

$$\nu = \frac{\omega_e}{\omega_e x_e}, \quad (57)$$

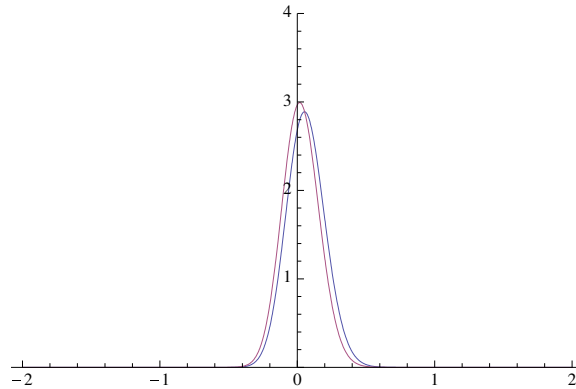


Figure 2. Graphs of $|\Psi^\nu(z, x; 0)|^2$ and $|\Phi^\nu(\mu, \sigma, x; 0)|^2$ for $z = 1, \mu = 0.02, \sigma = 0.13$.

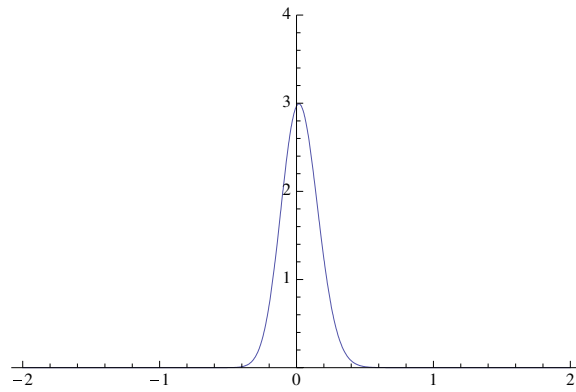


Figure 3. Graphs of $|\Psi^\nu(z, x; 0)|^2$ and $|\Phi^\nu(\mu, \sigma, x; 0)|^2$ for $z = 0.1, \mu = 0.0002, \sigma = 0.013$.

where ω_e and $\omega_e x_e$ are known as the molecular harmonic and anharmonicity constants, respectively. The values of these constants are available for known diatomic molecules in [3]. For the case of $^1\text{H}^{35}\text{Cl}$, $\nu \approx 57.44$ and $n_{\max} = 28$.

We can thus write the time-dependent density probabilities as

$$|\Psi^\nu(z, x; t)|^2 = \frac{1}{\mathcal{N}_0^\nu(|z|^2)} \sum_{n,m=0}^{27} \frac{\bar{z}^n z^m}{(\rho_n \rho_m)^{1/2}} e^{-\frac{i(E_n - E_m)}{\hbar} t} \psi_n^\nu(x) \psi_m^\nu(x) \quad (58)$$

and

$$|\Phi^\nu(\mu, \sigma, x; t)|^2 = \frac{1}{\mathcal{N}(\mu, \sigma)} \sum_{n=0}^{27} e^{-\frac{(n-\mu)^2}{2\sigma^2}} e^{-\frac{i(E_n - E_m)}{\hbar} t} \psi_n^\nu(x) \psi_m^\nu(x). \quad (59)$$

Two cases are given for illustration: $z = 1$ and $z = 0.1$. For each value of z , the parameters μ and σ are calculated from (50) and (51). The corresponding graphs are presented in figures 2 and 3 for $t = 0$. They indicate that a better localization is achieved when $z = 0.1$.

Moreover, the good behaviour of the time evolution of the generalized coherent states is shown in figure 4. A similar behaviour is produced with the Gaussian coherent states.

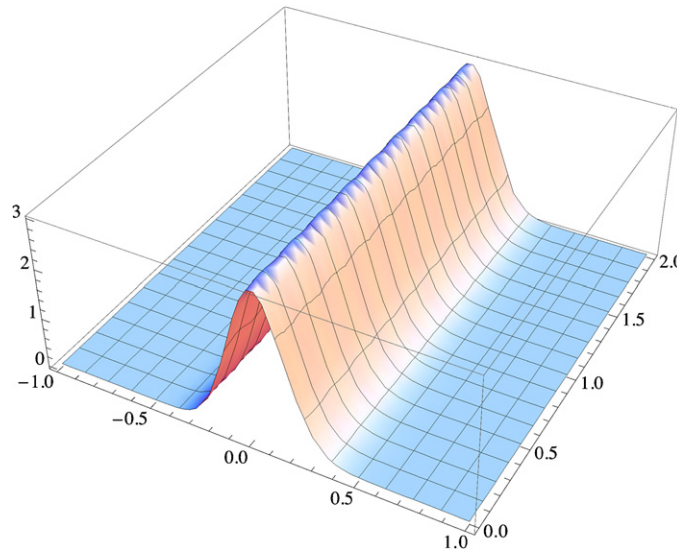


Figure 4. Graph of $|\Psi^\nu(z, x; t)|^2$ for $z = 0.1$, $(\beta x) \in [-1, 1]$, $(\frac{\hbar\beta^2}{m}t) \in [0, 2]$.

The computation of the dispersions Δx and Δp , requires to compute the following integrals (for the generalized coherent states, for example):

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} (\Psi^\nu(z, x; 0))^2 x^2 dx, \quad \langle x \rangle^2 = \left(\int_{-\infty}^{\infty} (\Psi^\nu(z, x; 0))^2 x dx \right)^2 \tag{60}$$

and

$$\begin{aligned} \langle p^2 \rangle &= - \int_{-\infty}^{\infty} \Psi^\nu(z, x; 0) \frac{d^2 \Psi^\nu(z, x; 0)}{dx^2} dx, \\ \langle p \rangle^2 &= \left(\int_{-\infty}^{\infty} \Psi^\nu(z, x; 0) \frac{d \Psi^\nu(z, x; 0)}{dx} dx \right)^2, \end{aligned} \tag{61}$$

which is done in practice by numerical integration (because the functions under the integral sign are rapidly decreasing to zero). For $z = 0.1$, we find

$$(\Delta x)^2 \approx 0.018, \quad (\Delta p)^2 \approx 14.01. \tag{62}$$

So we see that the dispersion is very small on the position and the product of the square of the dispersions is approximately 0.25 as expected from the Heisenberg uncertainty principle (56).

6. Conclusions and further work

We have presented an extension of recent results [11] on the behaviour of generalized and Gaussian coherent states for the case of a quantum system with a finite discrete energy spectrum. Our treatment of different ladder operators allows a verification of some algebra structures or factorization of the Hamiltonian. Our definition of generalized coherent states as some finite superpositions of energy eigenstates is closely related to the infinite case. A comparison of the behaviour of these states with the Gaussian ones which are defined independently of any algebra structure has led to a consistency of both approaches of coherent states.

Let us mention that, in our particular model of the anharmonic oscillator, different generalized coherent states may be constructed from (45). Indeed, with respect to the three types of ladder operators we have considered, we could also choose other values for ρ_n . For the states associated with the annihilation operator K_- , we have

$$\rho_n(k^\nu) = \prod_{i=1}^n i(v-i) = n! \frac{\Gamma(v)}{\Gamma(v-n)}, \quad (63)$$

while for the states associated with b^- , we have $\rho_n = n!$ as for the harmonic oscillator. Since we have $\rho_n(k^\nu) > \rho_n > n!$, it would be useful to compare those different generalized coherent states with the Gaussian ones having in mind that the parameters μ and σ have to be adjusted for each set of coherent states. Connections with both the harmonic oscillator and infinite well, in their corresponding limits, will be also relevant. The extension to a 2D Morse potential, and its relation with the infinite square well in 2D will be interesting as well being an example where degeneracies appear in the energy spectrum.

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References

- [1] Messiah A 1970 *Quantum Mechanics* (Amsterdam: North-Holland)
- [2] Landau L D and Lifshitz E M 1977 *Quantum Mechanics* (Oxford: Pergamon)
- [3] Herzberg G 1950 *Molecular Spectra and Molecular Structure I: Spectra of Diatomic Molecules* 2nd edn (New York: Van Nostrand)
- [4] Klauder J R 1960 *Ann. Phys.* **11** 123
- [5] Glauber R J 1963 *Phys. Rev.* **130** 2529
Glauber R J 1963 *Phys. Rev.* **131** 2766
- [6] Klauder J R and Skagerstam B S 1985 *Coherent States—Applications in Physics and Mathematical Physics* (Singapore: World Scientific)
- [7] Perelomov A M 1986 *Generalised Coherent States and Their Applications* (Berlin: Springer)
- [8] Klauder J R, Penson K A and Sixdernihiers J M 2001 *Phys. Rev. A* **64** 013817
- [9] Fernandez D J, Hussin V and Rosas-Ortiz O 2007 *J. Phys. A: Math. Gen.* **40** 6491
- [10] Fox R F and Choi M F 2001 *Phys. Rev. A* **64** 042104
- [11] Dello Sbarba L and Hussin V 2007 *J. Math. Phys.* **48** 012110
- [12] Nieto M N and Simmons L M 1979 *Phys. Rev. A* **19** 438
- [13] Dong S H, Lemus R and Frank A 2002 *Int. J. Quantum Chem.* **86** 433
- [14] Molski M 2006 *Eur. Phys. J. D* **40** 411
- [15] Nielsen M A and Chuang I L 2002 *Quantum Computation and Quantum Information* (Cambridge: Cambridge University Press)
- [16] Angelova M, Dobrev V K and Frank A 2001 *J. Phys. A: Math. Gen.* **34** L503
- [17] Angelova M, Dobrev V K and Frank A 2004 *Eur. Phys. J. D* **31** 27
- [18] Morse P M 1929 *Phys. Rev.* **34** 57
- [19] Ramakrishna V and Rabitz H *et al* 2000 *Phys. Rev. A* **61** 32106
- [20] Cordero R and Hojman J 1970 *Lett. Nuovo Cimento* **4** 1123
- [21] Kondo A E and Truax D R 1988 *J. Math. Phys.* **16** 862
- [22] Cooper I L 1993 *J. Phys. A: Math. Gen.* **26** 1601
- [23] Cooper I L and Gupta R K 1995 *Phys. Rev. A: At. Mol. Opt. Phys.* **52** 941
- [24] Aldaya V and Guerrero J 2005 *J. Phys. A: Math. Gen.* **38** 6939
- [25] Guerrero J and Aldaya V 2006 *J. Phys. A: Math. Gen.* **39** L267

- [26] Frank A and Van Isacker P 1994 *Algebraic Methods in Molecular and Nuclear Structure Physics* (New York: Wiley)
- [27] Iachello F and Levine R D 1995 *Algebraic Theory of Molecules* (Oxford: Oxford University Press)
- [28] Alhassid Y, Gürsey F and Yachello F 1983 *Ann. Phys.* **148** 346
- [29] Wu J and Alhassid Y 1990 *J. Math. Phys.* **31** 557
- [30] Englefield M J and Quesne C 1991 *J. Math. Phys.* **24** 3557
- [31] Frank A and Wolf K B 1984 *Phys. Rev. Lett.* **52** 1737
- [32] Berrondo M and Palma A 1980 *J. Phys. A: Math. Gen.* **13** 773
- [33] Frank A, Lemus R, Bijker R, Pérez-Bernal F and Arias J M 1996 *Ann. Phys.* **252** 211
- [34] Pérez-Bernal F, Arias J M, Frank A, Lemus R and Bijker R 1997 *J. Mol. Spectrosc.* **184** 1
- [35] Lemus R and Frank A 2003 *J. Phys. A: Math. Gen.* **36** 4901
- [36] Angelova M and Frank A 2005 *Phys. At. Nucl.* **68** 1625
- [37] Holstein T and Primakoff H 1940 *Phys. Rev.* **58** 1098
- [38] Aldaya V and Guerrero J 1995 *J. Math. Phys.* **36** 3191
Aldaya V and Guerrero J 2003 *J. Math. Phys.* **44** 5456
- [39] Oh P and Rim C 1997 *Mod. Phys. Lett. A* **12** 163
- [40] Guerrero J and Aldaya V 1999 *Mod. Phys. Lett. A* **14** 1689
- [41] Hussin V and Nieto L M 2005 *J. Math. Phys.* **46** 122102
- [42] Odake S and Sasaki R 2006 *J. Math. Phys.* **47** 102102