A simple approach to solve the time independent Schröedinger equation for 1D systems

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Abstract
A simple algebraic approach based on the well known angular momentum SU(2) algebra is presented to describe 1D systems for arbitrary potentials. The approach is based on the dimension increase of the 1D harmonic oscillator space through the addition of a scalar boson, keeping constant the total number of bosons. In this new space the realization of the coordinate and momentum correspond to components of the angular momentum algebra, which in turn define the coordinate and momentum representation bases. This remarkable result allows the Hamiltonian matrix representation to be expressed in terms of a diagonal matrix characterizing the potential we are considering. The solutions are obtained as an expansion of harmonic oscillator functions by purely algebraic means. As an example of our approach the Morse and asymmetric double Morse potentials are considered.

1. Introduction

The solutions of the time-independent Schröedinger equation are of primary importance in quantum mechanics. Since this is a differential equation the natural way to approach the solutions consists in applying the mathematical methods available to solve differential equations [1–3]. Besides the integro-differential techniques—regarded as the traditional approach—a route focused on the integrability of the systems represents a successful alternative [4]. The eigenvalue problem however can also be considered using factorization methods leading to algebraic techniques where only commutation relations are used to obtain the matrix representation of the Hamiltonian [5–7]. The representative example is given by the solutions for the 1D harmonic oscillator in second quantization [8]. In this case the wave functions as well as the Hamiltonian acquire a quite simple form in terms of bosonic operators and any observable depending on the coordinate and momentum can be realized in terms of the bosonic algebraic space. A similar situation is present for 2D and 3D harmonic oscillators, although with more elaborate treatments. In particular the advantage of dealing with an algebraic treatment for the 3D harmonic oscillator taking into account symmetry was extensively developed by M. Moshinsky [9].

Symmetry and dynamical groups are fundamental concepts in quantum mechanics. The symmetry group is defined as the maximal set of transformations that commutes with the Hamiltonian, an identification that in general is not trivial to find out [10, 11]. On the other hand the dynamical group embraces all the transformations that connect the whole space of eigenvectors [12]. For finite spaces like the bound states of the 1D Morse potential for instance, the dynamical group corresponds to the \( U(2) \) unitary group, a manageable compact group we are familiar with because of its relation with the angular momentum [13]. In contrast, for infinite spaces the dynamical groups are non-compact involving more sophisticated tools to deal with the analysis of the representations [14]. An example of the latter case corresponds precisely to the 1D harmonic oscillator system whose dynamical group is \( Sp(2, R) \) [12]. However it is still possible to set up a compact group as the dynamical group for the harmonic oscillator. This task is accomplish by adding an extra scalar boson to the harmonic oscillator space with the additional constraint of taking a fixed total number of bosons.

The addition of a scalar boson to generate a dynamical unitary group was introduced in 1974 by Arima and Iachello in the field of nuclear physics, where an s boson is added to the five dimensional harmonic oscillator to generate the \( U(6) \) group, leading to the Interacting Boson Model (IBM) [15, 16]. Latter on encouraged by the
success of the IBM model [16], the $U(4)$ algebraic model was proposed for describing molecular rotation-vibration spectra of diatomic molecules [17]. The $U(4)$ model consists in adding a scalar boson to the bosonic space of a 3D harmonic oscillator keeping the total number of bosons $N$ constant. In this context $N$ plays the role of a parameter connected with the depth of the potential, a fact that provides a description where anharmonicities are taken into account from the outset. A major advantage of this approach is the existence of dynamical symmetries: analytic solutions when only invariant operators associated with a given group chain is present in the Hamiltonian with a precise physical interpretation. In particular the $U(4) \supset SO(4) \supset SO(3)$ dynamical symmetry was associated with the solutions of a displaced Morse potential, an argument based on a mapping between the Morse and the $SO(4)$ states as well as on the displayed rotor spectrum [18–20]. A similar situation is present in the 2D case, where the dynamical group is $U(3)$ and two relevant dynamical symmetries emerge: the $U(2)$ and the $SO(3)$, associated with the 2D harmonic oscillator basis and a displaced oscillator respectively [21].

A similar approach adding a scalar boson was applied to the 1D harmonic oscillator giving rise to the $U(2)$ vibron model to describe the 1D vibrational degrees of freedom of molecules [22–24]. In this case the dimension of the symmetry group $U(1)$ is increased by one, generating the $U(2)$ group. Among the $U(\nu + 1)$ models, the $U(2)$ model is distinctive in the sense that the ladder operators for the Morse and Pöschl-Teller potentials can be identified with the generators of the $SU(2)$ group [13]. Consequently a mapping between the ladder operators (in configuration space) and the $U(2)$ unitary group can be established, with the clear identification of $N/2 = j$ as the number of bound states. This feature of the model led to the possibility to estimate the potential energy surfaces of molecules from vibrational spectroscopic analysis [13].

In this contribution we consider the $U(2)$ algebraic approach from a different perspective in order to provide a pedagogical viewpoint of the unitary group approach model presented in [25]. We start considering the ladder operators for the Morse potential in configuration space as well as their identification with the angular momentum commutation relations. After taking into account the linear approximation for the coordinate and momentum, the $U(1 + 1)$ space involving the addition of the scalar boson to the 1D space is introduced through the generators of the the group. This procedure allows the intuitive identification of the coordinate and momentum in the algebraic space. This is a non trivial result due to the fact that the receipt existing in second quantization to construct an observable in Fock space from configuration space does not work anymore in models where the scalar boson is involved. In order to reinforce the resulting connection between algebraic and configuration spaces we proceed to set up the connection from a formal point of view using a general minimization approach previously presented [26–28]. In addition the connection with the Holstein-Primakoff transformation is given. The search for this mapping leads to identify three bases, corresponding to the energy, coordinate and momentum representations without any reference to an specific potential. It is through the appropriate manipulations of these bases that it is possible to establish in a simple matrix form the stationary solutions of 1D Schrödinger equation. This feature of the model allows the Hamiltonian to be expressed in terms of a similitude transformation of a diagonal matrix of the potential trivially constructed in the position representation. We show that in principle this approach may be applied to any potential of a 1D system, albeit here we present the application for Morse and double Morse potentials. The Morse potential is considered because of its suitability to be treated with two different schemes, allowing the method to be evaluated in both energies and wave functions. Since the analytical solution are known the convergence in energies as well as in wave functions can be studied. On the other hand the double Morse potential is studied in the framework of a potential profile deformation as an example where analytical solutions are not known in general.

This article is organized as follow. Section 2 is devoted to present a summary of the algebraic treatment for the Morse oscillator in order to introduce the $SU(2)$ group associated with the bound states. In section 3 we revisit the procedure of adding an extra scalar boson to the bosonic harmonic oscillator space in order to set up the $U(2)$ dynamical group for 1D systems. Section 4 is devoted to identify the coordinates and momenta realizations in the algebraic space, a nontrivial step that leads to the energy, coordinate and momentum representations. This task is accomplished from different viewpoints, using the Morse ladder operators, the Holstein-Primakoff transformation as well as a formal minimization procedure. In section 5 the unitary group approach is introduced to obtain the algebraic representation of 1D systems associated with general potentials. Two examples corresponding to the Morse and double Morse potentials potentials are analyzed in section 6. Finally, in section 7 the summary and our conclusions are presented.

## 2. Ladder operators for the Morse oscillator

Before considering the unitary group approach we believe it is convenient to start recalling the 1D Morse potential characterized by the Hamiltonian
\[ H_M = \frac{1}{2\mu} \hat{p}^2 + D(1 - e^{-\beta(q - q_0)})^2, \]  
(1)

where \( D \) is the depth of the potential, \( q_0 \) the equilibrium position and \( \beta \) is related to the range of the potential. The solutions of corresponding Schrödinger equation are given by

\[ \langle q|\psi\rangle = N_j e^{-y^2/\beta^2} L_j^{(2j-v)}(y),\]

(2)

where \( L_j(y) \) are the associated Laguerre functions, the argument \( y \) is related to the physical displacement coordinate \( q \) by 

\[ y = (2j + 1)e^{-\beta q}, \]

while for the normalization constant

\[ N_j = \frac{\beta(2j - 2\nu)\Gamma(\nu + 1)}{\Gamma(2j - \nu + 1)}, \]

(3)

The eigenvalues are

\[ E_j(\nu) = \hbar\omega \left[ (\nu + 1/2) - \frac{1}{\kappa}(\nu + 1/2)^2 \right], \]

(4)

where \( \nu = 0, 1, \ldots, j - 1, \kappa = 2j + 1 \) and

\[ \omega = \sqrt{\frac{2D\beta^2}{\mu}}; \quad k = \frac{8D\mu}{\beta^2\beta^2}. \]

(5)

In analogy with the 1D harmonic oscillator system [8], it is possible to obtain the ladder operators \{ \( \hat{b}^\dagger, \hat{b} \) \} for the Morse functions (2) using the recurrence relations for the Laguerre polynomials with the following action [13, 29]:

\[ \hat{b}^\dagger|j\psi\rangle = k_+|j+1\psi\rangle; \quad k_+ = \sqrt{(\nu + 1)(1 - (\nu + 1)/\kappa)}, \]

(6a)

\[ \hat{b}|j\psi\rangle = k_-|j-1\psi\rangle; \quad k_- = \sqrt{\nu(1 - \nu/\kappa)}, \]

(6b)

\[ \hat{\varphi}|j\psi\rangle = \psi|j\psi\rangle. \]

(6c)

from which the following SU(2) commutation relations are obtained

\[ [\hat{b}, \hat{b}^\dagger] = 1 - \frac{2\kappa}{\nu}; \quad [\hat{\varphi}, \hat{b}^\dagger] = \hat{b}^\dagger; \quad [\hat{\varphi}, \hat{b}] = -\hat{b}, \]

(7)

and \( \hat{\varphi} = j - \hat{f}_0 \), with the relation to the angular momentum generators given by \( \{ \hat{b}^\dagger = \hat{J}_- / \kappa, \hat{b} = \hat{J}_+ / \kappa \} \). In terms of these ladder operators the momentum up to second order takes the form [30]

\[ \hat{p} = \frac{i}{2\sqrt{2\hbar\omega}} \left\{ f \hat{b}^\dagger + \frac{1}{\sqrt{\kappa}} g^* \hat{b} \right\} + H.c., \]

(8)

while for the Morse coordinate

\[ \frac{\gamma}{\beta} = \sqrt{\frac{\hbar}{2\omega\mu}} \left\{ f^*_d \frac{\hat{J}_d}{\sqrt{\kappa}} + (f \hat{b}^\dagger + \frac{1}{\sqrt{\kappa}} g^* \hat{b} \hat{b}^\dagger) + H.c. \right\}, \]

(9)

where the functions \( g^*_d, f_d, g_d \) are quantum number dependent functions given in [13, 30]. For large but finite \( \kappa \) the coordinate and momentum may be approximated as

\[ \hat{p} \approx \frac{i}{2\sqrt{2\hbar\omega}} \left\{ \hat{b}^\dagger - \hat{b} \right\} = \frac{i}{2\sqrt{2\hbar\omega}} \left\{ \hat{J}_- - \hat{J}_+ \right\}, \]

(10a)

\[ \frac{\gamma}{\beta} \approx q \approx \sqrt{\frac{\hbar}{2\omega\mu}} \left\{ \hat{b}^\dagger + \hat{b} \right\} = \sqrt{\frac{\hbar}{2\omega\mu}} \left\{ \hat{J}_+ + \hat{J}_- \right\}. \]

(10b)

In the approximation of large \( \kappa \) both coordinates and momenta are linear in the SU(2) generators. This fact allows the connection with the unitary group approach as we next explain.

### 3. The \( U(2) \) algebraic approach

In this section we present the main ingredients characterizing the \( U(2) \) unitary group approach. To accomplish this goal we start presenting the salient features characterizing the 1D harmonic oscillator.

#### 3.1. 1D harmonic oscillator

Let us start considering the 1D harmonic oscillator with reduced mass \( \mu \) and frequency \( \omega \). The Hamiltonian in configuration space is
with eigenfunctions \[ \psi_n(q) = N_n e^{-\frac{q^2}{2\lambda_0^2}} H_n(q/\lambda_0), \] and normalization constant \[ N_n = (\pi^{1/2} \lambda_0^{-\frac{1}{2}})^{-1}, \] where \( \lambda_0 = \sqrt{\hbar/(\omega \mu)} \) corresponds to the length unit. The Hamiltonian as well as the eigenfunctions can be translated into the Fock space through the introduction of the bosonic creation \( a^\dagger \) and annihilation \( a \) operators with the usual relations

\[
 a^\dagger = \frac{1}{\sqrt{2}} \left( \sqrt{\frac{\mu_\omega}{\hbar}} q - i \frac{P}{\sqrt{\hbar \omega \mu}} \right), \quad a = \frac{1}{\sqrt{2}} \left( \sqrt{\frac{\mu_\omega}{\hbar}} q + i \frac{P}{\sqrt{\hbar \omega \mu}} \right)
\]

Hence in Fock space the Hamiltonian takes the form

\[
 \hat{H}_{\text{Fock}}^{\text{h.o.}} = \hbar \omega (\hat{n} + 1/2),
\]

with \( \hat{n} = \hat{a}^\dagger \hat{a} \) and eigenkets

\[
 |n\rangle = \frac{1}{\sqrt{n!}} (a^\dagger)^n |0\rangle.
\]

The matrix elements of the coordinates and momenta can be calculated through the basic matrix elements

\[
 \langle n+1|\hat{a}^\dagger|n\rangle = \sqrt{n+1}; \quad \langle n-1|\hat{a}|n\rangle = \sqrt{n},
\]

given the inversion of (14):

\[
 q = \frac{1}{\sqrt{2}} \sqrt{\frac{\hbar}{\omega \mu}} (\hat{a}^\dagger + \hat{a}); \quad p = \frac{i}{\sqrt{2}} \sqrt{\hbar \omega \mu} (\hat{a}^\dagger - \hat{a}).
\]

Notice the resemblance of (10) with (18). Indeed in the harmonic limit

\[
 \lim_{\kappa \to \infty} \hat{b}^\dagger = \hat{a}^\dagger; \quad \lim_{\kappa \to \infty} \hat{b} = \hat{a},
\]

and both expansions coincide.

Suppose now that we are interested in describing a 1D system using a harmonic oscillator basis \( |n\rangle \). The first problem is that the dimension of the basis is infinity and as a consequence

\[
 \sum_{n=0}^{\infty} |n\rangle \langle n| = 1.
\]

In practice when the basis is cut off, the closure condition (20) is not satisfied. The question which arises is the following: it is possible to use a harmonic oscillator basis recovering in some way the closure condition? The importance of this question is evident and the answer is based on the introduction of the scalar boson previously mentioned. We shall see that an additional boson \( s \) - whose meaning is not clear- solves the problem as long as the total number of bosons \( N \) is kept constant. \( N \) labels the finite space where the mathematical description of any 1D system is described and it basically establishes the dimensionality of the space of harmonic oscillator functions to be considered.

In the next section we introduce the unitary group approach identifying the physical bosons with \( t^\dagger(t) \) instead of the usual one \( a^\dagger(a) \). The different names are introduced in order to set up clearly the different roles they play in the algebraic space.

### 3.2. \( U(2) \)- algebraic space

The \( U(2) \) space is established by adding the scalar boson \( s^\dagger(s) \) to the space of physical bosonic operators \( t^\dagger(t) \)-called \( \hat{a}^\dagger(\hat{a}) \) in the previous section- with the constraint that the total number of bosons \( N \) is preserved. The bilinear products satisfy the commutations relations associated with the generators of the \( U(2) \) group [7]. A convenient form to express the generators is

\[
 G_{U(2)} = \{ \hat{N} = t^\dagger t + s^\dagger s, \hat{n} = t^\dagger t, t^\dagger s, s^\dagger t \}.
\]
elements. Another alternative is based on the realization of the Morse ladder operators and their connection with the SU(2) generators common to the U(2) algebraic approach. The ultimate connection method consists in a minimization approach where the best description is obtained as an expansion of the generators of the dynamical group. In this contribution all of them are discussed.

In the algebraic space the total number of bosons specifies a representation space labeled by the totally symmetric representation $[N]$ of the $U(2)$ group, enclosing the possible eigenvectors for any 1D system. In the familiar angular momentum language the connection of $N$ with the angular momentum $j$ is given by $N = 2j$. A convenient realization of the angular momentum generators in the algebraic space (21) is

$$\hat{J}_x = \frac{1}{2}(s^+s + s^-s); \quad \hat{J}_y = -\frac{i}{2}(s^+s - s^-s); \quad \hat{J}_z = \frac{1}{2}(s^+s - s^-s).$$

(22)

Any operator is expected to be expressed in terms of these generators. A convenient basis should be selected by choosing a complete set of commuting operators composed of $\hat{J}^2$ and any of the components (22). In particular we can label the states with the eigenvalues associated with the operators $\hat{J}_x$. In this case the eigenstates acquire the simple form

$$|[N]n\rangle = \frac{1}{\sqrt{(N-n)!n!}} (s^+)^{N-n}(s^+)^{n}|0\rangle,$$

(23)

satisfying the eigensystem

$$\hat{J}_x|[N]n\rangle = \frac{N}{2} ([N]n + 1)|[N]n\rangle,$$

$$\hat{J}_z|[N]n\rangle = (n - \frac{N}{2})|[N]n\rangle.$$  

(24a, 24b)

Because of the property (24) it is said that the kets are associated with the chain of groups $U(2) \supset U(1)$. (25)

The importance of this basis stems from the fact that the physical number of bosons appears as an invariant operator that defines the basis. Using the same algebraic manipulation for the 1D harmonic oscillator it is possible to obtain in a straightforward way the matrix elements of the generators (21):

$$\hat{N}|[N]n\rangle = N |[N]n\rangle,$$

$$\hat{n}|[N]n\rangle = n |[N]n\rangle,$$

$$\hat{t}^s|[N]n\rangle = \sqrt{(N-n)(n+1)} |[N]n + 1\rangle,$$

$$\hat{s}^t|[N]n\rangle = \sqrt{(N-n+1)n} |[N]n - 1\rangle.$$  

(26a, 26b, 26c, 26d)

The fact that the $U(2)$ group is the dynamical group of any 1D system means that any dynamical variable in configuration space may be translated into the algebraic space. The question which arises is how to establish the mapping between the spaces.

4. Coordinate and momentum representations

The introduction of the scalar boson in the unitary group approach makes difficult to establish the connection with configuration space. In this section we present several arguments that leads to the same algebraic realizations of the coordinate and momentum. We start with an heuristic argument.

Let us consider the normalized generators

$$\hat{b}^\dagger \equiv \frac{t^s}{\sqrt{N}}; \quad \hat{b} \equiv \frac{s^t}{\sqrt{N}}.$$  

(27)

From (26c) and (26d) we immediately obtain

$$\hat{b}^\dagger |[N]n\rangle = \sqrt{(n+1)(1 - n/N)} |[N]n + 1\rangle,$$

$$\hat{b}|[N]n\rangle = \sqrt{n (1 - (n - 1)/N)} |[N]n - 1\rangle.$$  

(28a, 28b)

These expressions resemble the harmonic oscillator matrix elements (17) except for the anharmonic corrections going as $n/N$, which vanish in the $N'$ large limit with finite $n$. This feature suggests the mapping

$$\hat{a}^\dagger \rightarrow \hat{b}^\dagger; \quad \hat{a} \rightarrow \hat{b},$$

(29)
to translate the expressions (18) into the algebraic space with coordinate \( \hat{Q} \) and momentum \( \hat{P} \) given by

\[
\hat{Q} = \frac{1}{\sqrt{2}} \sqrt{\hbar \mu} \left( \hat{b}^+ + \hat{b} \right); \quad \hat{P} = \frac{i}{\sqrt{2}} \sqrt{\hbar \omega} \left( \hat{b}^+ - \hat{b} \right),
\]

which according to the matrix elements (28) satisfy

\[
q = \lim_{N \to \infty} \hat{Q}; \quad p = \lim_{N \to \infty} \hat{P},
\]

for fixed \( n \). The identification (30) was obtained using heuristic arguments linked with the behavior of the matrix elements (28) in the harmonic limit. We next present a second argument based on the algebraic realization of the Morse coordinate and momentum previously presented and suggested by the resemblance between (6) and (28).

4.1. Morse potential and unitary group approach

From section 2 we have that for the Morse potential the realization of the coordinate and momentum in the linear approximation takes the form (10)

\[
\hat{p} = \frac{i}{2} \sqrt{2 \hbar \omega \mu} \left\{ \frac{j_+ - j_-}{\sqrt{\kappa}} \right\}, \quad (32a)
\]

\[
\gamma \approx q = \frac{\hbar}{2 \omega \mu} \left\{ \frac{j_+ + j_-}{\sqrt{\kappa}} \right\}, \quad (32b)
\]

where the operators \( j_{\pm} \) act over the space of Morse kets \( |j\nu\rangle \) with finite \( j \). On the other hand we have that from the SU(2) realization (22) the ladder operators are

\[
j_+ = j_x + i j_y = t^* s; \quad j_- = j_x - i j_y = s t. \quad (33)
\]

The substitution of these expressions into (32) allows the following identification

\[
\hat{p} \to \hat{p} = \frac{i}{2} \sqrt{2 \hbar \omega \mu} \frac{1}{\sqrt{N + 1}} \{s^* t - t^* s\}, \quad (34a)
\]

\[
\gamma \approx q \to \hat{Q} = \frac{\hbar}{2 \omega \mu} \frac{1}{N + 1} \{t^* s + s^* t\}, \quad (34b)
\]

where we have taken into account the relation \( \kappa = N + 1 \). The resulting expressions (34) are now defined in the U(2) unitary group space and they basically coincide with (30) except for the fact that for the Morse realizations \( N \) is finite, a fact we proceed to investigate. To accomplish this goal we calculate the commutation relations

\[
[\hat{Q}, \hat{P}] = i\hbar \left( 1 - \frac{2\hbar}{N} \right). \quad (35)
\]

In the limit \( N \to \infty \) for fixed \( n \) the usual commutation relations are recovered, a fact that suggests the need to take the infinite limit in the U(2) approach. If this is the case \( N \approx \kappa \) and indeed (34) coincides with (30).

Two arguments leading to the realizations (30) have been given. We next present a formal argument based on a minimization approach supporting such mapping.

4.2. Minimization approach

In this section we shall follow the general approach presented in [26–28] where given a \( U(\nu + 1) \) unitary group space a procedure to establish a correspondence between operators in configuration and algebraic spaces is given. We start by establishing the mapping

\[
|N|n \leftrightarrow |n\rangle; \quad n = 0, 1, \ldots, N, \quad (36)
\]

which is based on the fact that the basis (23) represents a finite harmonic oscillator space containing the physical boson \( t \). In addition the density operator is introduced

\[
\hat{\rho} = \sum_{n=0}^{N} p_n |n\rangle \langle n| \approx \sum_{n=0}^{N} p_n \ |N|n \rangle \langle N|n\rangle, \quad (37)
\]

with normalization \( \sum_{n=0}^{N} p_n = 1 \). We now address the problem of establishing an algebraic realization of a general operator \( \hat{f}_V \) in configuration space. Since we have established the mapping involving the harmonic oscillator functions, it is enough to propose the linear expansion [26]

\[\text{Notice that to describe the system in equilibrium with thermal bath at temperature } T, \text{ we can use } p_n = Z^{-1} e^{E_n/\kappa T} \text{ with } Z = \sum e^{E_n/\kappa T}. \]
where \( \hat{Y}_s \) are generators of the \( U(2) \) group and the coefficients \( \alpha^{(m)}_s(\mathcal{F}_s) \) are determined with the criterion that they are to be the best given the proposed expansion (38). Here we are interested in \( \hat{F}_s \), identified with coordinates and momenta. The coefficients \( \alpha^{(m)}_s(\mathcal{F}_s) \) are obtained by solving the a set of equations obtained from the following minimization procedure.

Let \( \Delta \) the operator corresponding to the difference between the exact operator \( \hat{F}_s \) and the algebraic approximation:

\[
\hat{\Delta} = \hat{F}_s - \sum_t \alpha_t(\mathcal{F}_s) \hat{Y}_t,
\]

The error of the approximation, \( \epsilon \), is estimated by calculating the average of \( \hat{\Delta} \hat{\Delta}^\dagger \):

\[
\epsilon = \text{Tr}(\hat{\Delta} \hat{\Delta}^\dagger).
\]

The coefficients \( \alpha_t \)'s are obtained by minimizing the error

\[
\frac{\partial \epsilon}{\partial \alpha_r} = 0; \quad \forall r,
\]

which leads to the set of equations [26]

\[
\sum_t \alpha_t(\mathcal{F}_s) \text{Tr}(\hat{\rho} \hat{Y}_t \hat{Y}_t^\dagger) = \text{Tr}(\hat{\rho} \hat{F}_s \hat{F}_s^\dagger).
\]

Introducing explicitly the density operator we have

\[
\sum_t \alpha_t(\mathcal{F}_s) \sum_{n=0}^N p_n(\mathcal{N} n) \hat{Y}_t \hat{Y}_t^\dagger(\mathcal{N} n) = \sum_{n=0}^N p_n(\mathcal{N} n) \hat{F}_s \hat{F}_s^\dagger(\mathcal{N} n).
\]

Notice that because of the mapping (36) to determine the action of the operator \( \hat{F}_s \), we make the substitution \( n \rightarrow |n\rangle \). Let us now identify the coordinates \( q \) and momenta \( p \) with the operator \( \hat{F}_s \), while \( \hat{Q} \) and \( \hat{P} \) with \( \hat{\Delta} \) respectively. In accordance with the selection rules involved in the matrix elements (17) as well as (26) we shall consider a linear expansion in terms of the generators

\[
Y_1 = t^s s, \quad Y_2 = s^t t.
\]

We now contemplate the physical situation where in the distribution of states the ground state dominates, a fact that it is taken into account by considering

\[
p_0 = 1 - \epsilon; \quad p_1 = \epsilon,
\]

and taking the limit \( \epsilon \to 0 \). The result is

\[
\hat{Q} = \frac{i}{\sqrt{2\omega\mu}} \left[ t^s s + s^t t \right], \quad \hat{P} = \frac{i}{\sqrt{2\omega\mu}} \left[ t^s s - s^t t \right],
\]

which coincide with (30). This is the formal justification of the algebraic realization of the coordinate and momentum given by (30). We now proceed to obtain an equivalent result using the Holstein-Primakoff transformation [31].

### 4.3. Holstein-Primakoff transformation

Here we regard the connection of our treatment with the Holstein-Primakoff transformation, widely used to restrict the space of harmonic oscillator states [31]. Given the generators of the \( SU(2) \) group in terms of the realization (22) we again build the ladder operators (33), which turn out to be basically the operators defined in (27). The action of these operators over the \( U(1) \) basis (23) is given by (26) and recast in the following form

\[
\hat{J}_+|\mathcal{N} n \rangle = \sqrt{\mathcal{N}} \sqrt{(1 - n/\mathcal{N})} \sqrt{(n + 1)} \mathcal{N} n + 1 \rangle,
\]

\[
\hat{J}_-|\mathcal{N} n \rangle = \sqrt{\mathcal{N}} \sqrt{(1 - (n - 1)/\mathcal{N})} \mathcal{N} n - 1 \rangle.
\]

These matrix elements can be reproduced in the context of the harmonic oscillator basis \(|n\rangle\) by taking the following realization for the ladder operators

\[
\hat{J}_+ = \sqrt{\mathcal{N}} \sqrt{(1 - (\bar{n} - 1)/\mathcal{N})} t^s,
\]

\[
\hat{J}_- = \sqrt{\mathcal{N}} \sqrt{(1 - \bar{n}/\mathcal{N})} t^s,
\]
with \( \hat{n} = t^\dagger t \). These expressions constitute the Holstein-Primakoff transformation with \( N = 2j \). If we now invert (48) and carry out the substitution into the coordinates and momenta (18), we obtain

\[
q = \frac{1}{\sqrt{2}} \sqrt{\frac{\hbar}{\omega \mu}} \frac{1}{\sqrt{N}} (\hat{J}_z (1 - \hat{n}/N)^{-1/2} + \hat{J}_y (1 - (\hat{n} - 1)/N)^{-1/2}); \tag{49a}
\]
\[
p = i \frac{1}{\sqrt{2}} \sqrt{\frac{\hbar \omega \mu}{2}} \frac{1}{\sqrt{N}} (\hat{J}_z (1 - \hat{n}/N)^{-1/2} - \hat{J}_y (1 - (\hat{n} - 1)/N)^{-1/2}), \tag{49b}
\]
which correspond to a state dependent expansions. In the region where \( x = n/N \ll 1 \), the first term in the Taylor series expansion of \( (1 - x)^{-1/2} \) dominates and the approximation \( (1 - x)^{-1/2} \approx 1 \) may be taken to be applied in (49), leading to our identification (46).

### 4.4. Hamiltonian

We have shown four methods that led to the identification (30). From all of them the minimization argument is the most convincing because of its formality based on the physical argument of the ground state dominance in a Boltzman distribution.

Let us now return to the algebraic representation of the Hamiltonian (11). The anharmonization procedure

\[
p \rightarrow \hat{P}; \quad q \rightarrow \hat{Q},
\]

equivalent to (29) provides the algebraic Hamiltonian

\[
\hat{H}^{(2)}_{\text{alg}} = \frac{1}{2\mu} p^2 + \frac{\omega^2 \mu}{2} Q^2. \tag{51}
\]

This expression can be recast in more convenient form by noticing that

\[
\hat{Q} = \frac{1}{\sqrt{2}} \sqrt{\frac{\hbar}{\omega \mu}} \frac{2j_z}{\sqrt{N}}; \quad \hat{P} = -i \frac{1}{\sqrt{2}} \sqrt{\frac{\hbar \omega \mu}{2}} \frac{2j_y}{\sqrt{N}}. \tag{52}
\]

Substitution of (52) into the Hamiltonian (51), gives rise to

\[
\hat{H}^{(2)}_{\text{alg}} = \frac{\hbar \omega}{N} (\hat{J}_z^2 + \hat{J}_y^2) = \frac{\hbar \omega}{N} (\hat{J}^2 - \hat{J}_z^2), \tag{53}
\]

where we have used \( \hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 \) in the last part of the equation. If in addition we take into account that

\[
\hat{J}_z^2 = \frac{\hat{N}}{2} \left( \frac{\hat{N}}{2} + 1 \right), \tag{54}
\]

the Hamiltonian acquires the simple form

\[
\hat{H}^{(2)}_{\text{alg}} = \hbar \omega \left( \hat{n} + \frac{1}{2} - \frac{n^2}{N} \right). \tag{55}
\]

A remarkable consequence of this Hamiltonian is that it is diagonal in the \( U(1) \) basis (23):

\[
\hat{H}^{(2)}_{\text{alg}} \ket{N} n = E_n \ket{N} n, \tag{56}
\]

with eigenvalues

\[
E_n = \hbar \omega \left( n + \frac{1}{2} - \frac{n^2}{N} \right). \tag{57}
\]

Hence we say that chain (25) is associated with the energy representation with eigenkets (23). Hamiltonian (55) contains an anharmonic contribution characterized by the term \( 1/N \). A peculiar behavior of this spectrum is its degeneracy. Since \( n = 0, 1, \ldots, N \), a double degeneracy appears for both even and odd values of \( N \). The spectrum is reproduced twice, in a similar way to the \( U(2) \) model when applied to the Morse spectrum. However, for fixed \( n \), the anharmonic correction vanishes in the harmonic limit:

\[
\lim_{N \to \infty} \hat{H}_{\text{alg}}^{(4)} = \hat{H}_{\text{Hick}}. \tag{58}
\]

This is true as long as a finite subspace is considered.

We are now in position to interpret the three chains associated with the \( U(2) \) group:

\[
U(2) \supset U(1), \tag{59a}
\]
\[
U(2) \supset SO(2), \tag{59b}
\]
\[
U(2) \supset S\tilde{O}(2). \tag{59c}
\]
Chain (59) is characterized by the invariant operator \( \hat{J}_z = (2\hat{n} - \hat{N}) / 2 \) and because of (55) we say that it is associated with energy representation (or harmonic oscillator basis). Chains (59b) and (59c) are characterized by the invariants \( \hat{J}_x \) and \( \hat{J}_y \), respectively, and because of the relations (32) we can assert that chain (59b) provides the basis where the coordinate is diagonal

\[
\hat{J}_x |N\{\zeta\} = \zeta |N\{\zeta\} ; \quad \zeta = -\frac{N}{2}, -\frac{N}{2} + 1, \ldots, \frac{N}{2},
\]

while chain (59c) gives the basis where the momentum is diagonal

\[
\hat{J}_y |N\{\zeta\} = \bar{\zeta} |N\{\bar{\zeta}\} ; \quad \bar{\zeta} = -\frac{N}{2}, -\frac{N}{2} + 1, \ldots, \frac{N}{2}.
\]

Hence the bases \(|N\{\zeta\}\rangle\) and \(|N\{\bar{\zeta}\}\rangle\) are the coordinate and momentum representations, respectively. This is summarized in table 1.

The three bases in table 1 are complete and equivalent; any of them may be used to obtain the matrix representation of an arbitrary operator in the \( U(2) \) space. On the other hand both coordinate and momentum representations can be expressed in terms of the energy basis

\[
|N\{\zeta\}\rangle = \sum_{n=0}^{N} \langle [N]n|N\{\zeta\} \rangle |[N]n\rangle, \tag{62a}
\]

\[
|N\{\bar{\zeta}\}\rangle = \sum_{n=0}^{N} \langle [N]n|N\{\bar{\zeta}\} \rangle |[N]n\rangle. \tag{62b}
\]

The involved transformation coefficients may be obtained numerically by diagonalizing the matrix representation of the operators \( \hat{J}_x \) or \( \hat{J}_y \), respectively, but also analytically [32]. From figure 1 of [25] the coefficients are expected to be connected with rotations given in terms of Wigner’s matrices [32].

Because of the mapping (36) we are able to obtain a position representation of both kets in (62). For the coordinate representation (62a) for instance we have

\[
\langle \hat{q}|N\{\zeta\}\rangle = \sum_{n=0}^{N} \langle [N]n|N\{\zeta\} \rangle \langle \hat{q}|[N]n\rangle, \tag{63}
\]

where \( \hat{q} \) is chosen to be in units of \( \sqrt{\hbar/m}\). To illustrate the behavior of the bases in the position representation (62) we consider \( N = 100 \), corresponding to \( N + 1 \) harmonic oscillator functions [25]. In the first row of figure 2 of [25] the coordinate and momentum representations for the states \(|[N]0\rangle\), \(|[N]1\rangle\) are displayed. In this case both functions are real. Since the momentum representation is in general complex, the other cases correspond to the absolute value of the coordinate states (62a) for the cases \( \zeta = \pm 30, \pm 50 \) at the left panels, and the absolute value of momentum states \( \bar{\zeta} = \pm 30, \pm 50 \) for the right panels. The range of the states are basically established by \( \sqrt{N} \), in this example 10, as clearly noticed by the states \( \zeta = \pm N/2 \), which correspond to the maximum values of \( \zeta \). As \( \zeta \) decrease the number of nodes increases one by one, until the maximum of oscillations is reached at \( \zeta = 0 \). The states in coordinates representation establish the coordinate range we are considering in our description given \( N \). A remarkable result supporting the correct identification of the representations is the uncertainty principle. When in the coordinate representation the states are localized in a certain region, in the momentum representation a complementary behavior is present, a behavior supporting the identification (50).

### 5. Algebraic representation of 1D systems

Let us now consider a general Hamiltonian in configuration space

\[
\hat{H}_{\text{cs}} = \frac{1}{2\mu} \hat{\mathbf{p}}^2 + V(q). \tag{64}
\]

The corresponding algebraic Hamiltonian is obtained applying the anharmonization correspondence (50). A straightforward way to apply our approach would consist in introducing the transformation brackets associated with both coordinates and momenta. Following this approach, the Hamiltonian in the energy representation
takes the form:

$$H^{(E)} = W^t \Lambda^{(E)} W + T^t \Lambda^{(V)} T,$$

(65)

where $\Lambda^{(E)}$ corresponds to the diagonal contribution of the kinetic energy

$$||\Lambda^{(E)}|| = \hbar \omega \left( \frac{2}{N} \right) \delta_{\phi, \phi},$$

(66)

and $\Lambda^{(V)}$ the diagonal matrix associated with the potential

$$||\Lambda^{(V)}|| = \hbar \omega \left( \frac{1}{\sqrt{2}} \sqrt{\frac{\hbar}{\mu \omega}} \right) \frac{2 \zeta}{\sqrt{N}} \delta_{\phi, \phi},$$

(67)

The $T$ matrix stands for the transformation coefficients (62a) given by $T = || [N| \zeta]|N|n ||$, while $W$ for the transformation coefficients (62b) corresponding to $W = || [N| \zeta]|N|n ||$. The problem with this approach is that the spectrum turns out to be degenerate and it is not clear how to remove the spurious states. In order to elucidate an approach to identify the spurious states we proceed in the following form. We start adding and subtracting a quadratic term in such a way that the harmonic oscillator term

$$H_{\text{alg}}^{(E)} = \hbar \omega \left( \frac{n + 1}{2} - \frac{n^2}{N} \right) + \eta V^1(\hat{Q}).$$

(68)

where

$$V^1(Q) = -\frac{\omega^2 \mu}{2} \hat{Q}^2 + V(Q),$$

(69)

with $\eta$ being a control parameter in the interval $[0, 1]$, whose variation allows the potential to be transformed from a harmonic oscillator ($\eta = 0$) to the arbitrary potential $V(Q)$ ($\eta = 1$). Taking into account from (60) that the coordinate is diagonal in the position representation

$$\langle [N| \zeta]|\hat{Q}|[N| \zeta] \rangle = \frac{1}{\sqrt{2}} \sqrt{\frac{\hbar}{\mu \omega}} \frac{2 \zeta}{\sqrt{N}} \delta_{\phi, \phi},$$

(70)

the matrix elements of the Hamiltonian in the energy representation takes the form [25]

$$H^{(E)} = \Lambda^{(E)} + \eta T^t \Lambda^{(Q)} T,$$

(71)

where $\Lambda^{(E)}$ the diagonal contribution of the deformed harmonic oscillator

$$||\Lambda^{(E)}|| = \hbar \omega \left( \frac{n + 1}{2} - \frac{n^2}{N} \right) \delta_{\phi, \phi},$$

(72)

and $\Lambda^{(Q)}$ is the diagonal matrix of the potential $V(Q)$ in the position representation:

$$||\Lambda^{(Q)}|| = \hbar \omega \left[ -\frac{\zeta^2}{N} + \frac{1}{\hbar \omega} \left( \frac{1}{\sqrt{2}} \sqrt{\frac{\hbar}{\mu \omega}} \frac{2 \zeta}{\sqrt{N}} \right) \right] \delta_{\phi, \phi}.$$

(73)

In this scheme the matrix $W$ is not involved, and $T$ is calculated once and for all for a given $N$, while the diagonal matrix $\Lambda^{(Q)}$ is modified in accordance with the specific potential. The contribution (72) involves accidental degeneracy due to the quadratic term. This degeneracy manifests in the full Hamiltonian (71) by the appearance of degeneracy for the bound states in the $N$ large limit. This degeneracy is removed by substituting the diagonal term (72) by [25]

$$\left( n + \frac{1}{2} - \epsilon \frac{n^2}{N} \right); \text{ with } \epsilon = 1 \text{ for } n < N/2; \quad \epsilon = 0 \text{ for } n \geq N/2.$$

(74)

This form of removing the degeneracy although apparently arbitrary is based on a detail study of the eigenstates [25].

6. Examples

We now consider two examples to show the features of our approach. We first consider the Morse potential in order to appreciate the two algebraic forms to describe the same system in the framework of the $U(2)$ algebra. As a second example we study the asymmetric double Morse potential [33, 34] for different parameters as an example of potential profile deformation considered in catastrophe theory [35].
6.1. Morse potential

In accordance with section 2 the wave functions and energies for the Morse potential are given by (2) and (4) respectively. In terms of the generators the Hamiltonian takes the simple form

\[ \hat{H} = \frac{\hbar \omega}{2} \left( b^\dagger b + b b^\dagger + \frac{1}{4\kappa} \right), \]

where we recall that \( \kappa = 2j + 1 \) is finite and related with the depth of the potential through (5). In this scheme \( \kappa \) fixes the dynamical space of the bound states.

On the other hand, with the identification (34) the coordinates and momenta move to the \( U(2) \) space with commutation relations (35). The Hamiltonian (75) is not valid anymore and the Hamiltonian (1) must be considered. The basis to be considered is \( \hat{n} \) with \( N \) large. The advantage of this new point of view is that now any 1D potential may be considered independent of the potential as we next discuss.

Let us consider the Morse potential in the unitary group approach where the Hamiltonian matrix representation is given by (71). In the framework of the modified potential (69) the diagonal matrix (73) takes the form

\[ ||A^{(0)}|| = \hbar \omega \left[ -\frac{\zeta^2}{N} + \bar{D} \left( 1 - e^{-\beta \left( \frac{\zeta}{\sqrt{N} (\sqrt{\kappa} - \eta) \sqrt{\kappa} - 1) \right )} \right) \right] \delta_{\kappa',\kappa}, \]

with \( \zeta \) given by the spectrum (60), where for the sake of simplicity we have taken \( \hbar \omega \) and \( \sqrt{\hbar / (\omega \mu)} \) for energy and length units respectively. In this case we have the relations

\[ \beta = \frac{1}{\sqrt{2D}}; \quad \kappa = 4\bar{D}, \]

where the bar refers to dimensionless coordinates.

As a particular system we consider the following parameters for the Morse potential:

\[ \bar{D} = 3.75; \quad j = 7; \quad \kappa = 15; \quad \beta = \frac{1}{\sqrt{7.5}}, \]

with eigenvalues

\[ E_v = (v + 1/2) - \frac{1}{\kappa} (v + 1/2)^2. \]

Taking \( N = 1500 \), the diagonalization of the Hamiltonian matrix (71) leads to the correlation diagram displayed in figure 1 as a function of \( \eta \). On the other hand in table 2 we present the eigenvalues and its comparison with the exact energies. The convergence can be measured through the fidelity \( F \) or overlap of eigenstates involving different parameters \( N \). Calling \( \psi_{\alpha}^{(N)} \) the \( \alpha \)-th state we may demand \( F = |\langle \psi_{\alpha}^{(N)} | \psi_{\alpha}^{(N')} \rangle | \) to be as close to unit as we want for a given step \( \Delta = N' - N \). This approach should be followed when the exact solutions are not known [25]. In our case however we know the analytical solutions and consequently the wave functions are able to be directly compared.
In our approach the $\alpha$-th eigenstate takes the form
\[
|\psi^{(N)}_\alpha\rangle = \sum_{n=0}^{N} |nN\rangle |\psi^{N}_{\alpha n}\rangle |Nn\rangle.
\]
We shall obtain the corresponding position representation in order to carry out a direct comparison with the exact solutions. As noticed the wave function are very well described with the exception of the last bound states, whose tail for large distances is difficult to reproduce. However a larger value for $N$ may be chosen in order to get the precision we want in both energies and wave functions.

We should mention the importance of having selected $\bar{q}_0 = 0$ in the description of the Morse functions. The basis is given by harmonic oscillators functions centered at the origin and consequently as we move away from the origin a larger basis is needed to obtain the convergence. Consequently it is more efficient to select a null displacement and thereafter apply the displacement operator in terms of the momentum operator.

6.2. Asymmetric double Morse potential

In this section we study the solutions of the asymmetric double Morse potential (ADMP) defined by
\[
\hat{H} = \frac{\hat{p}^2}{2\mu} + D_1(1 - e^{-\beta_1(q+q_0)})^2 + D_2(1 - e^{\beta_2(q-q_0)})^2,
\]
which when translated into the algebraic space in the form (68) in units of $\hbar\omega$ for the energy and $\sqrt{\hbar/\mu\omega}$ for the length, takes the form
\[
\hat{H}_{alg}^{U(2)} = \left( \frac{\hat{p}^2}{2\mu} + \frac{1}{2} - \frac{1}{N} \hat{n}^2 \right) + \left[ \frac{-\hbar^2}{N} + \tilde{D}_1(1 - e^{-\tilde{\beta}_1(\sqrt{N}/\sqrt{N} + \tilde{q}_0)})^2 + \tilde{D}_2(1 - e^{\tilde{\beta}_2(\sqrt{N}/\sqrt{N} - \tilde{q}_0)})^2 \right],
\]
where here
\[
\tilde{D}_i = \frac{D_i}{\hbar\omega}; \quad \tilde{\beta}_i = \beta_i \sqrt{\hbar/\mu\omega}; \quad i = 1, 2.
\]
Let us now consider the ADMP analyzed in [25] with the parameters
\[
\tilde{D}_1 = 10; \quad \tilde{D}_2 = 4; \quad \tilde{\beta}_1 = 1; \quad \tilde{\beta}_2 = 0.8,
\]
for different values for the displacement parameter $\tilde{q}_0$ in order to analyze a potential profile deformation as depicted in figure 3. In terms of the matrix representation (71) the contribution $\Lambda^{(Q)}$ takes the form
\[
||\Lambda^{(Q)}(\tilde{q}_0)|| = \left[ \frac{-\hbar^2}{N} + \tilde{D}_1(1 - e^{-\tilde{\beta}_1(\sqrt{N}/\sqrt{N} + \tilde{q}_0)})^2 + \tilde{D}_2(1 - e^{\tilde{\beta}_2(\sqrt{N}/\sqrt{N} - \tilde{q}_0)})^2 \right] \delta_{\alpha,\tilde{\alpha}},
\]
where we have shown explicitly the $\tilde{q}_0$ dependence of the potential. The first potential I with $\tilde{q}_0 = 3$, corresponds to a potential well with two asymmetric minima. The second potential II has been chosen with $\tilde{q}_0 = 1.5$ is a case where the maximum and the nearest minimum merge resulting in an inflection point with a horizontal tangent. The potentials III and IV correspond to potentials wells of one minimum. The reason why this potential profile deformation is analyzed is because of its association with catastrophe theory [35].

In table 3 the first eight energies are displayed for the four potentials depicted in figure 3. A reasonable convergence is obtained with $N = 450$ for both energies and eigenstates. We notice the quantum mechanical behavior concerning the energy spacing which decreases with the potential broad. Since the solutions are given as an expansion in the $N$-dimensional space of harmonic oscillator functions it is straightforward to depict them. In figure 4 the first six wave functions are displayed for potentials I, II and III. In this case in order to evaluate the

| Table 2. Comparison between the exact bound Morse energies and the ones provided by the $U(2)$ model referred to the ground state. The parameters were taken to be (78) with $N = 1500$. |
|-----------------|--------|--------|--------|--------|--------|--------|
| Exact energy   | 0.8667 | 1.6    | 2.2    | 2.667  | 3.0    | 3.2    |
| $U(2)$ Model   | 0.8659 | 1.5973 | 2.1944 | 2.6576 | 2.9878 | 3.1873 |

955.3x841.9
convergence the wave functions with $N = 500$ was also calculated providing basically the same plots. We have thus obtain the the eigensystem for the potential profile in a straightforward way through the expression (71).

7. Conclusions

We have presented the unitary group approach to obtain the solutions of 1D systems. This is a simple algebraic approach where only the matrix elements (26) are directly involved and where no integrals are carried out. We started by introducing the algebraic realization of the Morse potential since the ladder operators obtained in configuration space satisfy the $SU(2)$ commutation relations. Later on the $U(2)$ approach was presented through the introduction of the scalar $s$ boson. The fact that both descriptions involves the $SU(2)$ algebra allows the

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.eps}
\caption{Comparison between exact and calculated Morse functions using (71) with parameter $N = 1500$.}
\end{figure}
connection of the coordinates and momenta with the algebraic space to be set up giving rise to the expressions (30). This result represented an heuristic argument which was reinforced with a formal minimization procedure [26]. To accomplish this task the mapping between the 1D harmonic oscillator functions and the basis (23) was established. The appropriate selection weights in the density operator corresponding to a dominance of the ground state leads to the identification (46) for the coordinates and momenta in the linear approximation, which turns out to be identical when heuristic and Holstein-Primakoff analysis are applied. A remarkable result is that it is by considering the \( N \) large limit that the coordinates and momenta satisfies the correct commutation relation, a behavior in contrasts to previous analysis of the algebraic models where \( N \to \infty \) represents the classical limit [36].

As a consequence of the identification (46) the bases associated with chains (59) render a precise meaning: the \( U(1) \) basis corresponds to the energy representation (harmonic oscillator basis), while the \( SO(2) \) and \( S\Omega(2) \) bases correspond to the coordinate and momentum representations respectively. This is an outstanding result that allows the matrix representation of any operator to be obtained in energy, coordinate or momentum representations. As a consequence the matrix representation of a 1D Hamiltonian in the energy representation can be obtained using the transformation coefficients connecting the coordinate and energy representations. The parameter \( N \) establishes the dimension of the space of harmonic oscillator functions. This

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**Figure 3.** Asymmetric double Morse potentials associated with different displacement parameter \( \bar{q}_0 \) and their corresponding eigenvalues. The potential I represents a well with two minima. The potential II presents only one minimum with an inflection point. The potential wells III and IV present one minimum.

**Table 3.** First 8 energies for the asymmetric double Morse potentials depicted in figure 3 taking \( N = 450 \).

| Level | I     | II    | III   | IV    |
|-------|-------|-------|-------|-------|
| 1     | 2.057 | 8.484 | 6.778 | 3.153 |
| 2     | 5.433 | 11.435| 9.491 | 8.330 |
| 3     | 7.024 | 12.823| 11.544| 13.770|
| 4     | 7.777 | 14.198| 13.873| 19.470|
| 5     | 8.476 | 15.975| 16.519| 25.392|
| 6     | 9.159 | 18.010| 19.424| 31.491|
| 7     | 10.018| 20.261| 22.551| 37.724|
| 8     | 11.056| 22.699| 25.867| 44.047|

---
feature provides a simple purely algebraic method to obtain the solutions of the 1D time-independent Schrödinger equation in terms of a harmonic oscillator basis.

The matrix representation (71) is given in terms of two diagonal matrices together with the transformation brackets. The calculation of the transformation brackets is independent of the potential and hence they are calculated only once for a given $N$. The diagonal matrix $\Lambda^{(E)}$ corresponding to the harmonic oscillator is trivially calculated and fixed for any system, while $\Lambda^{(Q)}$ is the diagonal matrix in the coordinate representation of the modified potential (69), which is also easily constructed. Hence this approach represents a friendly method to study systems where the analytical solutions of the Schrödinger equations are either not known or difficult to obtain by integration methods as long as the harmonic oscillator basis is suitable for the system considered.

**Figure 4.** First six wave functions for the asymmetric double Morse potential for the three selections of the displacement coordinate $q_0 = 3, 1.5, 1$. The total number of bosons was taken to be $N = 450$ in all cases.
As a test of our approach we have studied two systems, namely: Morse and asymmetric double Morse potentials (ADMP). Since analytical solutions for the Morse potential are known, its analysis represents a benchmark to test the convergence of this approach. Both energies and wave functions are reproduced in the $N$ large limit. In addition the ADMP has also been studied. In this case the analytical solutions are in general not known. This show the usefulness of our approach which, being easy to apply, is able to obtain the solutions of the time independent equation for 1D systems.

This approach may be useful in catastrophe theory where a small change in the original stable potential changes the topology of the problem [35]. This explain the application of our approach to the study of potential profile deformation. An outstanding feature of our approach is its generalization to 2D and 3D systems, although in a non trivial way due to the appearance of the angular momentum [37, 38].

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