Virial ansätzte for the Schrödinger Equation with a symmetric strictly convex potential. Part II.

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Abstract

Recently was introduced in the literature a procedure to obtain ansätze, free of parameters, for the eigenfunctions of the time-independent Schrödinger equation with symmetric convex potential. In the present work, we test this technique in regard to $x^2\kappa$-type potentials. We study the behavior of the ansätze regarding the degree of the potential and to the intervening coupling constant. Finally, we discuss how the results could be used to establish the upper bounds of the relative errors in situations where intervening polynomial potentials.

Keywords: ansatz, ansätze, virial theorem, Schrödinger, Fisher, monomial potentials.

1 Introduction

Since only a few quantum-mechanical models admit of exact solutions, approximations of diverse types constitute the tools for to treat with the Schrödinger Equation (SE). On the other hand, the Virial Theorem (VT) provides an extremely useful tackle for to study a quantum-mechanical system. In its non-relativistic quantum version, it is based on the SE. It relates the expectation value of the kinetic energy of the system to the expectation value of the directional derivative of the interaction potential that intervening in the Hamiltonian which describes the system [1]. Since it allows making conclusions about some interesting problems without solving the SE, since the 60s, hypervirial theorems [2, 3] have been gainfully incorporated into the literature. Furthermore, the subject was revisited in the Information Theory context, via the strong link between Fisher’s Information Measure (FIM) and the SE. In a nutshell, such connection is based upon the fact that a constrained minimization of the FIM leads to a SE-like equation [4-6]. This, in turn, implies intriguing relationships between various aspects of the SE, on the one hand, and the formalism of statistical mechanics as derived from the Jaynes’s Maximum Entropy Principle, on the other hand [7-14]. In particular, some fundamental consequences of the SE, such as the Hellmann-Feynman and Virial theorems, can be re-interpreted in terms of a special kind of reciprocity relations between relevant physical quantities similar to the ones exhibited by the thermodynamics’ formalism [7]. This demonstrates that a Legendre transform structure underlies the non-relativistic SE [8]. As a direct consequence of this Legendre-symmetry that underlies the connection between the FIM and the SE, an ansatz for the ground state eigenfunction of a SE with convex even informational-potential was derived [15]. Then, in a quantum scenario, as a direct consequence of the VT and symmetry considerations, a procedure to construct ansätze for the eigenfunctions of the SE with
symmetric convex potential, was developed \cite{16}. The technique leads to the exact eigenfunctions of the harmonic oscillator, and it was successfully tested regarding the quartic anharmonic oscillator \cite{16}. In the present communication, the formalism introduced in \cite{16} is applied to $x^{2\kappa}$-type potentials. We study the behavior of the ansätze in regard to the degree of the potential and to the intervening coupling constant. Considering scaling properties, we show that the relative error $\epsilon_n$ in the energy eigenvalue $E_n$ not depend on the coupling constant. To illustrate the properties of the ansatz-solutions, we consider the quantum pure quartic oscillator and compare the results with those obtained by computational numerical calculation. Then we describe the principal characteristics that present oscillators of greater degree. Finally, we discuss how these results could be used to establish the upper bounds of the relative errors in situations where intervening polynomial potentials.

2 Preliminaries

2.1 The quantum scenario

Let us consider the time-independent one-dimensional Schrödinger wave equation (SE) in dimensionless form,

$$\left[ -\frac{1}{2} \nabla_x^2 + U(x) \right] \psi_n(x) = E_n \psi_n(x), \quad \nabla_x^2 \equiv \frac{d^2}{dx^2},$$

where $U(x)$ stands for a time-independent symmetric convex real potential \cite{17}. In this one-dimensional scenario, the virial theorem states that \cite{1}

$$\langle -\nabla_x^2 \rangle_n = \langle x U'(x) \rangle_n,$$

where the expectation values are taken between stationary states of the Hamiltonian. For one-dimensional scenarios, $\psi_n$ is real \cite{18}, then the VT can be written as

$$-\int_{-\infty}^{\infty} \psi_n(x) \nabla_x^2 \psi_n(x) \, dx = \int_{-\infty}^{\infty} \psi_n^2(x) \, x U'(x) \, dx.$$

2.2 Virial ansätze for the eigenfunctions of the Schrödinger equation

Let $U$ be a real, symmetric and strictly convex potential which achieves its minimum at $x = \xi$. Then, from the VT and considering the symmetry property of the potential, ansätze $\chi_n$ for the eigenfunctions $\psi_n$ of the SE are constructed \cite{16}. They are given by

$$\chi_n(x) = \varphi_n(x) \chi_v(x),$$

where the $\chi_v$-function is defined by

$$\chi_v(x) = N \, e^{-g(x)},$$

with

$$g(x) = \begin{cases} -\int \sqrt{(x-\xi) U'(x)} \, dx & \text{if } \ x < \xi, \\ +\int \sqrt{(x-\xi) U'(x)} \, dx & \text{if } \ x \geq \xi, \end{cases}$$

the constant $N$ determined by normalization condition and the functions $\{\varphi_n, n = 0, 1, 2, \ldots\}$ chosen as a set of orthonormal polynomials with weight function $\sigma(x) = \chi_v^2(x)$,

$$\langle \varphi_i \varphi_j \rangle_\sigma = \int_{-\infty}^{\infty} \varphi_i(x) \varphi_j(x) \, \sigma(x) \, dx = \delta_{ij}.$$
The explicit form of the sequence \( \{ \varphi_n, n = 0, 1, 2, \ldots \} \) can be established from the Gram-Schmidt orthonormalization process \[19\]

\[
\varphi_0(x) = 1, \\
\varphi_n(x) = a_n \left[ (x - \xi)^n - \sum_{k=0}^{n-1} \langle (x - \xi)^n \varphi_k \rangle_\sigma \varphi_k(x) \right] \text{ for } n \geq 1,
\]

where

\[
\langle (x - \xi)^n \varphi_k \rangle_\sigma = \int_{-\infty}^{\infty} (x - \xi)^n \varphi_k(x) \sigma(x) \, dx,
\]

and the \( a_n \) are constants determined by the normalization condition \[7\]. Moreover, they can be expressed in terms of the Gram determinant \[19\].

Once we have at our disposal the ansätze for the eigenfunctions, we can obtain approximate energy eigenvalues,

\[
E_n \approx E_n^{\text{ansatz}} = \langle \chi_n | H | \chi_n \rangle = \left\langle \chi_n \bigg| -\frac{1}{2} \nabla_x^2 + U(x) \bigg| \chi_n \right\rangle.
\]

Furthermore, they can be calculated using the virial theorem \[2\],

\[
E_n^{\text{ansatz}} = \bigg\langle \chi_n \bigg| \frac{1}{2} (x - \xi) U'(x) + U(x) \bigg| \chi_n \bigg\rangle.
\]

### 2.3 The Quartic Anharmonic Oscillator

The Schrödinger equation for a particle of unit mass in a quartic anharmonic potential reads

\[
\left[ -\frac{1}{2} \nabla_x^2 + \frac{1}{2} \omega^2 x^2 + \lambda x^4 \right] \psi_n = E_n \psi_n, \quad \lambda \geq 0,
\]

where \( \lambda \) is the coupling constant.

The characteristics of the potential allow applying the technique cited above. The \( \chi_v \)-function \[16\] is given by \[16\]

\[
\chi_v(x) = N \exp[-g(x)] = N \exp \left\{ \frac{\omega^3}{12\lambda} \left[ 1 - \left( 1 + \frac{4\lambda}{\omega^2} x^2 \right)^{3/2} \right] \right\},
\]

where \( N \) is determined by the normalization condition. The ansätze \( \{ \chi_n \} \) for the eigenfunctions \( \{ \psi_n \} \) are given by \[4\] with \( \chi_v \) given by \[13\] and, being \( \{ \varphi_n \} \) a family of orthonormal real polynomials associated to the weight function \( \sigma(x) = \chi_v^2(x) \), which can be obtained using \[8\].

The approximate energy eigenvalues \[11\] are given by

\[
E_n \approx E_n^{\text{ansatz}} = \omega^2 \langle x^2 \rangle_n + 3\lambda \langle x^4 \rangle_n,
\]

where the expectation values are evaluated in respect to the ansätze \( \chi_n \) for the eigenfunctions \( \psi_n \).

The ansatz curves for several sets of the coupling constant values can be observed in \[16\]. There they were compared with the eigenfunctions curves numerically obtained. The curve associated with the ground state is bell-shaped. It is observed that for small values of \( \lambda \left( \lambda \lesssim \omega^2/2 \right) \) both curves overlap.
but, as the value of \( \lambda \) grows, the width of the bell corresponding to the eigenfunction decreases a little faster than that of the curve corresponding to the ansatz. This difference propagates to the excited states. In the other hand, the approximate energy eigenvalues were compared with the numerical ones. Consistently the results show that, for small values of \( \lambda \) the relative errors in the energy eigenvalues \( \epsilon_n \) are small \( (\epsilon_n \lesssim 1\%) \). When \( \lambda \) increases, \( \epsilon_n \) increases. The question is, are these relative errors bounded? We will return to this matter later.

3 Quantum oscillator with a \( x^{2\kappa} \)-type potential.

In this section, we show the results obtained when dealing with monomial potentials. We are interested in the behavior of the ansätze, in regard to the degree of the potential and to the intervening coupling constant. Besides the practical relevance of these potentials in connection with several areas of science, the results obtained here are going to be a useful tool to assess the applicability of the procedure in more complex situations.

For reasons of clarity, in this section we will deal with even potentials. The ansatz solutions for symmetric potentials regarding \( x = \xi \) can be obtained performing the translation transformation \( x \rightarrow x - \xi \) in the obtained solutions for even potentials [16].

3.1 Ansätze for \( x^{2\kappa} \)-type potential

Consider the Schrödinger equation for a particle of unit mass, given by

\[
\left[ -\frac{1}{2} \nabla_x^2 + \lambda_\kappa x^{2\kappa} \right] \psi_n^{(\kappa)}(x) = E_n^{(\kappa)} \psi_n^{(\kappa)}(x), \quad \kappa \in \mathbb{N}, \quad \lambda_\kappa > 0. \quad (15)
\]

The potential and its derivatives are given by

\[
U_\kappa(x) = \lambda_\kappa x^{2\kappa}, \quad U'_\kappa(x) = 2\kappa \lambda_\kappa x^{2\kappa - 1}, \quad U''_\kappa(x) = 2\kappa(2\kappa - 1)\lambda_\kappa x^{2\kappa - 2}. \quad (16)
\]

Immediately, we observe that \( U_\kappa \) is a symmetric and strictly convex function[17], with a unique minimum at \( x = 0 \),

\[
\forall x \in \mathbb{R}, \quad U_\kappa(-x) = U_\kappa(x), \quad U'_\kappa(0) = 0, \quad U''_\kappa(x) \geq 0. \quad (17)
\]

Then, the characteristics of the potential allow applying the technique cited in the previous section.

We start by constructing the virial \( \chi_v \)-function. Considering (16) we can write

\[
\int \sqrt{x U'_\kappa(x)} dx = \sqrt{2\kappa \lambda_\kappa} \int |x|^{\kappa} dx = \begin{cases} -\frac{\sqrt{2\kappa \lambda_\kappa}}{\kappa + 1} |x|^ {\kappa+1} & \text{for } x < 0 \\ +\frac{\sqrt{2\kappa \lambda_\kappa}}{\kappa + 1} |x|^{\kappa+1} & \text{for } x \geq 0 \end{cases}. \quad (18)
\]

Substituting (18) in (6) we get

\[
g(x) = \frac{\sqrt{2\kappa \lambda_\kappa}}{\kappa + 1} |x|^{\kappa+1}, \quad (19)
\]

and the \( \chi_v \)-function (5) is given by

\[
\chi_v^{(\kappa)}(x) = N_\kappa \exp \left[ -\frac{\sqrt{2\kappa \lambda_\kappa}}{\kappa + 1} |x|^{\kappa+1} \right]. \quad (20)
\]
Enforcing the normalization condition, we obtain
\[ N_\kappa = \frac{1}{\sqrt{I_o^{(\kappa)}}} \left[ \frac{2\sqrt{2\kappa \lambda_\kappa}}{\kappa + 1} \right]^{1/[2(\kappa+1)]}, \quad I_o^{(\kappa)} = \int_{-\infty}^{\infty} e^{-|x|^{\kappa+1}} dx. \] (21)

The virial weight function is given by
\[ \sigma_\kappa(x) = \left[ \chi_\kappa^{(\kappa)}(x) \right]^2 = N_\kappa^2 \exp \left[ \frac{2\sqrt{2\kappa \lambda_\kappa}}{\kappa + 1} |x|^{\kappa+1} \right]. \] (22)

The ansatz \( \chi_n^{(\kappa)} \) for the eigenfunction \( \psi_n^{(\kappa)} \) can be written as
\[ \chi_n^{(\kappa)}(x) = \varphi_n^{(\kappa)}(x) \chi_{\kappa}^{(\kappa)}(x), \] (23)
with the functions \( \{ \varphi_n^{(\kappa)}, n = 0, 1, 2, \ldots \} \) chosen as a set of orthonormal polynomials with weight function \( \sigma_\kappa(x) \) (22). Explicit expressions of them can be obtained using the Gram-Schmidt process (8). It is computationally advantageous to express \( \varphi_n^{(\kappa)} \) in terms of lower-order orthogonal polynomials using the three-term recurrence (19, 20). For the present case, we have
\[ \begin{align*}
\varphi_0^{(\kappa)} &= 1, \\
\varphi_1^{(\kappa)} &= \langle x^2 \rangle_{\sigma_\kappa}^{-1/2} x, \\
\varphi_n^{(\kappa)} &= \beta_n \left[ x \varphi_{n-1}^{(\kappa)} - \langle x \varphi_{n-1}^{(\kappa)} \varphi_{n-2}^{(\kappa)} \rangle_{\sigma_\kappa} \varphi_{n-2}^{(\kappa)} \right], \quad \text{for } n \geq 2,
\end{align*} \] (24)
where the \( \beta_n \) coefficients are given by
\[ \beta_n = \left[ \langle x^2 \varphi_{n-1}^{(\kappa)} \rangle_{\sigma_\kappa} - \langle x \varphi_{n-1}^{(\kappa)} \varphi_{n-2}^{(\kappa)} \rangle_{\sigma_\kappa} \right]^{-1/2}. \]

The approximate energy eigenvalues (11) are given by
\[ E_n^{(\kappa)} = \left\langle U_\kappa(x) + \frac{1}{2} x U'_\kappa(x) \right\rangle_n^{(\kappa)} = (\kappa + 1) \lambda_\kappa \left\langle x^{2\kappa} \right\rangle_n^{(\kappa)}, \] (25)
where \( \langle \quad \rangle_n^{(\kappa)} \) denoted that the expectation values are taken in respect to the ansätze \( \chi_n^{(\kappa)} \).

### 3.2 Behavior of the ansätze with the system parameters

The explicit polynomial expressions of the \( \varphi_n^{(\kappa)} \)-functions can be written as
\[ \varphi_n^{(\kappa)}(x) = \sum_{j=0}^{n} \alpha_{nj}^{(\kappa)} x^j, \] (26)
where the coefficients \( \alpha_{nj}^{(\kappa)} \) can be calculated from the Gram-Schmidt orthonormalization process (10, 11). Immediately, one can distinguish between even and odd orthonormal polynomial, \( \alpha_{nj}^{(\kappa)} = 0 \) when the parity of \( n \) is different from the parity of \( j \). The not null coefficients can be expressed in terms of the ground state moments,
\[ \alpha_{nj}^{(\kappa)} = \alpha_{nj}^{(\kappa)} \left( \mu_0^{(\kappa)}, \mu_2^{(\kappa)}, \ldots, \mu_{2n}^{(\kappa)} \right), \] (27)
where
\[ \mu_{2i}^{(\kappa)} = \langle x^{2i} \rangle_{\sigma_{\kappa}} = \int_{-\infty}^{\infty} x^{2i} \sigma_{\kappa}(x) \, dx = \left( \frac{\kappa + 1}{2\sqrt{2\kappa\lambda_{\kappa}}} \right)^{2i/(\kappa+1)} J_{2i}^{(\kappa)}, \]  \tag{28}

with
\[ J_{2i}^{(\kappa)} = \frac{I_{2i}^{(\kappa)}}{I_{0}^{(\kappa)}}, \quad I_{2i}^{(\kappa)} \equiv \int_{-\infty}^{\infty} x^{2i} e^{-|x|^\kappa+1} \, dx. \]  \tag{29}

From (23) and (26), the ansatz \( \chi_{n}^{(\kappa)} \) for the eigenfunction \( \psi_{n}^{(\kappa)} \) can be written as
\[ \chi_{n}^{(\kappa)}(x) = \sum_{j=0}^{n} \alpha_{nj}^{(\kappa)} x^{j} \chi_{v}^{(\kappa)}(x), \]  \tag{30}

and the approximate energy eigenvalues (25) can be expressed as
\[ E_{n}^{(\kappa)} = (\kappa + 1) \lambda_{\kappa} \int_{-\infty}^{\infty} x^{2\kappa}\left[ \chi_{n}^{(\kappa)}(x) \right]^{2} \sigma_{\kappa}(x) \, dx = \]
\[ = (\kappa + 1) \lambda_{\kappa} \sum_{i,j=0}^{n} \alpha_{ni}^{(\kappa)} \alpha_{nj}^{(\kappa)} \int_{-\infty}^{\infty} x^{2\kappa} x^{i+j} \sigma_{\kappa}(x) \, dx = \]
\[ = (\kappa + 1) \lambda_{\kappa} \sum_{i,j=0}^{n} \alpha_{ni}^{(\kappa)} \alpha_{nj}^{(\kappa)} \langle x^{i+j+2\kappa} \rangle_{\sigma_{\kappa}}. \]  \tag{31}

Therefore, the energy eigenvalue \( E_{n}^{(\kappa)} \) depends on \( \lambda_{\kappa} \) and the first \( 2(n + \kappa) \) ground state moments,
\[ E_{n}^{(\kappa)} = E_{n}^{(\kappa)} \left( \lambda_{\kappa}, \mu_{0}^{(\kappa)}, \mu_{2}^{(\kappa)}, \ldots, \mu_{2(n+\kappa)}^{(\kappa)} \right). \]  \tag{32}

### 3.2.1 Scale transformation properties

We describe here the changes in the ansatz-solutions under a scaling transformation when intervenes a \( x^{2\kappa} \)-potential. For clarity, in the expressions of this section, we drop the subscripts or superscripts that indicate the degree of the potential.

It is well known that, under the scaling transformation \( x \rightarrow v = \lambda^{1/[2(\kappa+1)]} x \), the SE (15) takes the form
\[ \left[ -\frac{1}{2} \frac{d^{2}}{dv^{2}} + v^{2\kappa} \right] \psi_{n}^{sc}(v) = \mathcal{E}_{n} \psi_{n}^{sc}(v). \]  \tag{33}

The scaling transformation relation between the eigenfunctions and between the energy eigenvalues are given by (see Appendix)
\[ \psi_{n}(x) = \lambda^{1/[4(\kappa+1)]} \psi_{n}^{sc}(\lambda^{1/[2(\kappa+1)]} x), \quad E_{n} = \lambda^{1/(\kappa+1)} \mathcal{E}_{n}. \]  \tag{34}

\[ \star \text{ The scaling transformation of the ansätze} \]

Following the procedure of the last section, we obtain the virial function for the transformed SE (33),
\[ \chi_{v}^{sc}(v) = N^{sc} \exp \left[ - \frac{\sqrt{2\kappa}}{\kappa + 1} |v|^\kappa+1 \right]. \]  \tag{35}
Enforcing the normalization condition, we obtain

\[ N^{sc} = \frac{1}{\sqrt{I_0}} \left[ \frac{2 \sqrt{2 \kappa}}{\kappa + 1} \right]^{1/[2(\kappa+1)]} , \quad I_0 = \int_{-\infty}^{\infty} e^{-|v|^\kappa+1} dv . \]  

(36)

The ansatz \( \chi_n^{sc} \) for the eigenfunction \( \psi_n^{sc} \) is given by

\[ \chi_n^{sc}(v) = \varphi_n^{sc}(v) \varphi_v^{sc}(v) , \]  

(37)

where the orthonormal polynomials \( \varphi_n^{sc} \) associated to the virial weight function \( \sigma^{sc} = [\chi_v^{sc}]^2 \) have the form

\[ \varphi_n^{sc}(v) = \sum_{j=0}^n A_{nj} v^j , \]  

(38)

where the coefficients \( A_{ij} \) can be calculated using (8) and (9). The not null coefficients can be expressed in terms of the ground state moments,

\[ A_{nj}^{sc} = A_{nj}^{(sc)}(\mu_v^{sc}, \mu_2^{sc}, \cdots, \mu_{2n}^{sc}) , \]  

(39)

where

\[ \mu_{2i}^{sc} = \langle v^{2i} \rangle^{sc}_o = \int_{-\infty}^{\infty} v^{2i} \sigma^{sc}(v) dv = \left( \frac{\kappa + 1}{2 \sqrt{2 \kappa}} \right)^{2i/[(\kappa+1)]} J_{2i} , \]  

(40)

with \( J_{2i} \) given by (29). The relationship between the transformed moments (40) and the original ones (28) is given by

\[ \langle x^{2i} \rangle_{\sigma_v} = \lambda^{-i/[(\kappa+1)]} \langle x^{2i} \rangle^{sc}_{\sigma_v} . \]  

(41)

Considering (8) and (41), with a bit of algebra we obtain the relation between the expansion coefficients of the orthonormal polynomials \( \varphi_n \) and \( \varphi_v^{sc} \),

\[ \alpha_{nj} = A_{nj} \lambda^{i/[(2(\kappa+1)]} . \]  

(42)

Taking the relationship between the coefficients \( \alpha_{nj} \) and \( A_{nj} \) (42) into account, the inverse scaling transformation \( v \rightarrow x = \lambda^{-1/[2(\kappa+1)]} v \) leads to

\[ \chi_n^{sc}(\lambda^{1/[2(\kappa+1)]} x) = \varphi_n^{sc}(\lambda^{1/[2(\kappa+1)]} x) \varphi_v^{sc}(\lambda^{1/[2(\kappa+1)]} x) = \]

\[ = N^{sc} \left( \sum_{j=0}^n A_{nj} \lambda^{i/[(2(\kappa+1)]} x^j \right) \exp \left[ - \frac{\sqrt{2\kappa \lambda}}{\kappa + 1} |x|^\kappa+1 \right] = \]

\[ = N^{sc} \left( \sum_{j=0}^n \alpha_{nj} x^j \right) \exp \left[ - \frac{\sqrt{2\kappa \lambda}}{\kappa + 1} |x|^\kappa+1 \right] . \]  

(43)

Considering (20), (28) and (26), the above equation can be written as

\[ \chi_n^{sc}(\lambda^{1/[2(\kappa+1)]} x) = \frac{N^{sc}}{N} \varphi_n(x) \varphi_v(x) = \frac{N^{sc}}{N} \chi_n(x) . \]  

(44)
From (21) and (36) we have

$$\frac{N}{N_{sc}} = \lambda^{1/[4(\kappa+1)]}. \quad (45)$$

Finally, substituting (45) in (44) we get

$$\chi_n(x) = \lambda^{1/[4(\kappa+1)]} \chi_n^{sc}(\lambda^{1/[2(\kappa+1)]} x). \quad (46)$$

Therefore, taking (34) and (46) into account, we can assert that the ansatz satisfy the same scale transformation property that the eigenfunctions satisfy.

* The scaling transformation of the energy eigenvalues

Taking (23) into account, the approximate energy eigenvalues for the transformed SE (33) are given by

$$E_{\text{ans}}^n = \left\langle U_{sc}^{\kappa}(v) + \frac{1}{2} v [U_{sc}^{\kappa}]'(v) \right\rangle_n^{sc} = (\kappa + 1) \langle v^{2\kappa} \rangle_n^{sc}, \quad (47)$$

where the expectation values $\langle \rangle_n^{sc}$ are taken in respect to the ansatz $\chi_n^{sc}$ for the eigenfunction $\psi_n^{sc}$. Using (37) and (38), with $\sigma^{sc} = [\chi^{sc}]^2$, we have

$$E_{\text{ans}}^n = (\kappa + 1) \int_{-\infty}^{\infty} v^{2\kappa} [\varphi_n^{sc}(v)]^2 \sigma^{sc}(v) \, dv = (\kappa + 1) \sum_{i,j=0} A_{ni} A_{nj} \langle v^{i+j+2\kappa} \rangle_o^{sc}. \quad (48)$$

Then, considering (41) and (42), we can write

$$E_{\text{ans}}^n = (\kappa + 1) \lambda^{\kappa/(\kappa+1)} \sum_{i,j=0} \alpha_{ni} \alpha_{nj} \langle x^{i+j+2\kappa} \rangle_o. \quad (49)$$

Finally, taking (31) into account, we obtain

$$E_{\text{ans}}^n = \lambda^{-1/(\kappa+1)} E_n^{\text{ans}}. \quad (50)$$

Therefore, the approximate energy eigenvalues, calculate using the ansatz for the eigenfunction of the SE, satisfy the same scale transformation property that the energy eigenvalues satisfy (34),

$$E_{\text{ans}}^n = \lambda^{1/(\kappa+1)} E_n^{\text{ans}}. \quad (51)$$

3.2.2 Dependence of the relative errors on the coupling constant

Due to the scaling properties of the theory, the relative error in the ansatz-solution satisfies the following relation

$$\epsilon_n^\chi(x) = \frac{|\chi_n(x) - \psi_n(x)|}{\psi_n(x)} = \frac{|\chi_n^{sc}(v) - \psi_n^{sc}(v)|}{\psi_n^{sc}(v)} = \epsilon_n^{sc}(v), \quad (v = \lambda^{1/[2(\kappa+1)]} x), \quad (52)$$

and the relative error in the energy eigenvalues not depend on coupling constant,

$$\epsilon_n = \frac{|E_n^{\text{ans}} - E_n|}{E_n} = \frac{|E_n^{\text{ans}} - E_n|}{E_n}. \quad (53)$$
3.3 Numerical results

To evaluate the ansatz-solutions, we are going to compare them with the eigenfunctions, and corresponding energy eigenvalues, obtained by computational numerical calculation. We will deal below with the harmonic oscillator \((\kappa = 1)\), with the quartic quantum oscillator \((\kappa = 2)\) and we will discuss the main features for quantum oscillators with \(\kappa > 2\).

⋆ The Harmonic Oscillator

The Schrödinger equation for a particle of unit mass in a harmonic potential is given by,

\[
\left[-\frac{1}{2} \nabla_x^2 + \frac{1}{2} \omega^2 x^2 \right] \psi_n = E_n \psi_n .
\] (54)

We can observe that the potential is a convex even function with a unique minimum at \(x = 0\). It is a \(x^2\)-type potential with \(\kappa = 1\). This case was treated in \([16]\) where been shown that the ansätze match the exact eigenfunctions of the SE (54).

⋆ The Pure Quartic Oscillator

The Schrödinger equation for a particle of unit mass in a pure quartic potential is given by,

\[
\left[-\frac{1}{2} \nabla_x^2 + \lambda x^4 \right] \psi_n = E_n \psi_n .
\] (55)

We can observe that the potential is a convex even function with a unique minimum at \(x = 0\). It is a \(x^2\)-type potential with \(\kappa = 2\). From (20) and (21) with \(\kappa = 2\), the \(\chi_u\)-function is given by

\[
\chi_u(x) = \frac{1}{\sqrt{I_o}} \left(\frac{4}{3}\right)^{1/6} \lambda^{1/12} \exp \left[-\frac{2\sqrt{\lambda}}{3} |x|^3 \right], \quad I_o = \int_{-\infty}^{\infty} e^{-|x|^3} dx .
\] (56)

For clarity, in the above expression, we omit the \(\kappa\)-subscript and the \((\kappa)\)-superscript. Then, the ansätze \(\chi_n\) \((\ref{eq:ansatz})\) for the eigenfunctions \(\psi_n\) can be written as

\[
\chi_n(x) = \frac{1}{\sqrt{I_o}} \left(\frac{4}{3}\right)^{1/6} \lambda^{1/12} \varphi_n(x) \exp \left[-\frac{2\sqrt{\lambda}}{3} |x|^3 \right],
\] (57)

with the functions \(\{\varphi_n, n = 0, 1, 2, \ldots\}\) chosen as a set of orthonormal polynomials with weight function \(\sigma = \chi_u^2\), where \(\chi_u\) is given by \((56)\). Explicit expressions of them can be obtained using the Gram-Schmidt process \((\ref{eq:gram-schmidt})\). Furthermore, them can be expressed in terms of lower-order orthogonal polynomials using the three-term recurrence \((\ref{eq:three-term})\).

In each graph of figure 1, the first five eigenfunctions of the quartic oscillator for a given \(\lambda\)-value are represented. They were obtained by computational numerically calculation (Matslise program was used) and the corresponding curves are drawn with black dashed lines. The corresponding ansätze \((57)\) are represented in the same graph. Solid lines represent their curves (black for \(\chi_0\), red for \(\chi_1\), blue for \(\chi_2\), green for \(\chi_3\) and coral for \(\chi_4\)). The curve associated with the ground state is bell-shaped. It is observed that for this state, for all values of \(\lambda\) considered, the width of the bell corresponding to the ansatz is a little greater than that of the curve corresponding to the eigenfunction. Consequently, due to the normalization condition, the ansatz curve looks lower. This difference between the ground state curves propagates to the excited states.
From (25) with $\kappa = 2$, the approximate energy eigenvalues are given by

$$E_n \approx E_{ans}^n = 3 \lambda \langle x^4 \rangle_n,$$

where the expectation values are evaluated in respect to the ansatz $\chi_n$ (57).

In the tables 1 are tabulated the eigenvalues of energy corresponding to the eigenfunctions plotted in figure 1. In each table, in the first column are the principal quantum numbers. The values of the second column correspond to those energy eigenvalues that one finds in the literature, obtained via a numerical approach to the SE. The values of the third column, correspond to the approximate energy eigenvalues obtained using (58). The fourth column displays the associated percentage relative error $\epsilon_n$,

$$\epsilon_n = \frac{|E_{ans}^n - E_n|}{E_n} \times 100.$$ 

As we can observe, the percentage relative error for the ground state energy eigenvalue is of the order of 3.2%, and for the excited states, $n \geq 1$, they are of the order of 1.7%. Furthermore, the results obtained show that the relative errors do not depend on the values of $\lambda$, which was to be expected, according to (53).
Tables 1. Energy eigenvalues for the quartic oscillator for several \( \lambda \)-values.

| Parameter values: \( k = 2, \lambda = 0.1 \) | Parameter values: \( k = 2, \lambda = 0.5 \) |
|---|---|
| \( n \) | \( E_n \) | \( E_{ansatz}^{(n)} \) | \( \epsilon_n \) | \( n \) | \( E_n \) | \( E_{ansatz}^{(n)} \) | \( \epsilon_n \) |
| 0 | 0.31005176 | 0.31946222 | 3.12673 | 0 | 0.53018104 | 0.54675835 | 3.12673 |
| 1 | 1.11003113 | 1.12974622 | 1.68501 | 1 | 1.89983651 | 1.93184898 | 1.68501 |
| 2 | 2.21005838 | 2.21667262 | 1.67946 | 2 | 3.72784897 | 3.79045685 | 1.67946 |
| 3 | 3.69993424 | 3.64004600 | 1.73455 | 3 | 5.82237276 | 5.92336456 | 1.73455 |
| 4 | 4.75986276 | 4.83020944 | 1.68316 | 4 | 8.13091301 | 8.26776951 | 1.68316 |
| 5 | 6.21037929 | 6.31602813 | 1.70512 | 5 | 10.61918647 | 10.80025618 | 1.70512 |

Parameter values: \( k = 2, \lambda = 0.1 \)

| Parameter values: \( k = 2, \lambda = 1 \) | Parameter values: \( k = 2, \lambda = 1.5 \) |
|---|---|
| \( n \) | \( E_n \) | \( E_{ansatz}^{(n)} \) | \( \epsilon_n \) | \( n \) | \( E_n \) | \( E_{ansatz}^{(n)} \) | \( \epsilon_n \) |
| 0 | 0.66798626 | 0.68887235 | 3.12673 | 0 | 0.76465338 | 0.78856199 | 3.12673 |
| 1 | 2.39364401 | 2.43397719 | 1.68501 | 1 | 2.74003839 | 2.78620836 | 1.68501 |
| 2 | 4.69679538 | 4.77567638 | 1.67946 | 2 | 5.37648857 | 5.46784777 | 1.67946 |
| 3 | 7.33572999 | 7.46297170 | 1.73455 | 3 | 8.39714162 | 8.54297000 | 1.73455 |
| 4 | 10.24430846 | 10.41673681 | 1.68316 | 4 | 11.72680581 | 11.9218702 | 1.68316 |
| 5 | 13.37933656 | 13.60747014 | 1.70512 | 5 | 15.31551711 | 15.5766493 | 1.70512 |

\( \epsilon_n^{(k)} \approx 0.54 \epsilon_o^{(k)} \) for \( n \geq 3 \) \( \gamma_n^\kappa = \left[ 1 + \frac{\epsilon_n^\kappa}{100} \right]^{-1} \).

The Pure Oscillator with \( \kappa \geq 2 \).

For \( x^{2\kappa} \)-type potentials with \( \kappa \geq 2 \), the graphic representation of the ground state eigenfunction is a bell-shaped curve. It is found that for this state, as the value of \( \kappa \) grows, the width of the bell decreases faster than that of the bell corresponding to the ansatz. This discrepancy propagates to the excited states. Consequently, the relative errors in the energy eigenvalues increase as \( \kappa \) increases. Once again, the results obtained show that the relative errors \( \epsilon_n^{(k)} \) do not depend on the coupling constant \( \lambda \), according to (53). In table 2 are tabulated the percentage relative errors \( \epsilon_n^{(k)} \) for the ten first energy eigenvalues. Figure 2 shown the percentage relative error \( \epsilon_n^{(k)} \) as function of the principal quantum number \( n \). Each curve correspond to a value of \( \kappa \) (black for \( \epsilon_n^{(1)} \), red for \( \epsilon_n^{(2)} \), blue for \( \epsilon_n^{(3)} \), green for \( \epsilon_n^{(4)} \) and coral for \( \epsilon_n^{(5)} \)). As can be observed, \( \epsilon_n^{(k)} \) increases considerably as \( \kappa \) increases. The maximum relative error occurs for the ground state energy eigenvalue. Then, they decrease for \( n \geq 1 \), and stay approximately constant for \( n \gtrsim 3 \), \( \epsilon_n^{(k)} \approx 0.54 \epsilon_o^{(k)} \) for \( n \gtrsim 3 \). Furthermore, from (59) we can write

\[ E_n(\lambda) = \gamma_n^\kappa E_n^{\text{ansatz}}(\lambda), \quad \text{with} \quad \gamma_n^\kappa = \left[ 1 + \frac{\epsilon_n^\kappa}{100} \right]^{-1}. \]
4 Discussion and perspectives

The results obtained show that the procedure introduced in [16] does not lead to satisfactory results when it is applied to $x^{2\kappa}$-type potentials, with $\kappa \geq 2$. In the other hand, we show that the relative errors in the energy eigenvalues do not depend on the coupling constant (coefficient of the monomial potential). This suggests that the relative errors for monomial potentials can be incorporate into the theory for establishing the upper bounds of the errors when the procedure is applied to polynomial potentials. To shed some light on this comment, we are going to focus on the quartic anharmonic oscillator, which was treated in [16]. The ansätze are given by (13) and the approximate energy eigenvalues by (14). Let’s start by observing that for small values of $\lambda$ ($\lambda \ll \omega^2/2$), the ansätze tend to those of the harmonic oscillator and for large values of the anharmonicity constant ($\lambda \gg \omega^2/2$), they tend to the ansätze of the pure quartic anharmonic oscillator (57). We investigate the behavior of the energy eigenvalues with the values of $\lambda$. The first six energy eigenvalues, as functions of $\lambda$, are plotted in figure 3. The graphs corresponding to the solutions obtained by computational numerical calculation are plotted with dashed black lines and the ansätze are plotted with solid lines (black for $E_{0}^{\text{ans}}$, red for $E_{1}^{\text{ans}}$, blue for $E_{2}^{\text{ans}}$, green for $E_{3}^{\text{ans}}$, coral for $E_{4}^{\text{ans}}$ and violet for $E_{5}^{\text{ans}}$). We focus on each pair of curves for a given principal quantum number $n$ (ansatz-curve vs numerical-curve). As can be observed for small $\lambda$-values, the such curves are overlapping (figure 3, left hand), as $\lambda$ increases they go grow apart, and when $\lambda \gg \omega^2/2$ the spacing between them tends to a maximum constant value (figure 3, right hand). Then we studied the dependence of the relative errors with the $\lambda$-values. Figure 4 shows the percentage relative errors $\epsilon_n$ corresponding to the energy eigenvalues plotted in figure 3 (the same colors pattern was used). As can be observed, for each eigenstate with principal quantum number $n$, the $\epsilon_n$ depends on $\lambda$. For small values of $\lambda$, $\epsilon_n$ is small and tends to zero when $\lambda$ tends to zero, which is consistent with the fact that the potential tends to that of the harmonic oscillator for which the procedure leads to the exact eigenvalues of energy [16]. When $\lambda$ increases, $\epsilon_n$ increases tending to a maximum value $\epsilon_n^{\text{max}}$ for a theoretically infinite $\lambda$-value, which is consistent with the fact that when $\lambda$ is much greater than $\omega^2/2$, the harmonic part of the potential is negligible in front of the quartic contribution, and for the purely quartic potential the relative error is constant (depend on $n$ but not on the value of $\lambda$). These results suggest that the percentage relative errors for the pure quartic potential (see tables 1) can be considered as the maximum values of the relative errors in the energy eigenvalues of the quartic anharmonic oscillator,

$$\epsilon_n = \epsilon_n(\lambda) \leq \epsilon_n^{\text{max}}$$

Figure 3. First six energy eigenvalues as functions of $\lambda$-values ($\omega = 1$).
5 Conclusions

The process derived from the virial theorem has been employed to obtain ansätze for \(x^{2\kappa}\)-type potentials. We have found that the technique applied to high degree monomial potentials does not satisfactorily lead to the quantitative behavior of the system, since the relative errors increase considerably when the degree of the monomial potential increases. In the other hand, since the ansätze preserve the scaling properties of the Schrödinger equation, the relative errors in the energy eigenvalues not depend on the coefficient of the monomial potential. This property result helpful to estimate the error bounds when the technique is applied to polynomial potentials. We took a first step in this line, we study the behavior of the quartic harmonic oscillator with its parameters. The results suggest that, the procedure introduced in provide satisfactory ansätze when it is applied to symmetric convex polynomial potentials, in which the largest of the polynomial coefficients is the one corresponding to the second degree term. Researches directed to establishing the error bounds as functions of the polynomial coefficients are in progress and will be reported elsewhere.

Appendix: Scale transformation of the Schrödinger equation.

We describe here the theory-changes under a scaling transformation for the SE given by

\[
\left[-\frac{1}{2}\frac{d^2}{dx^2} + \lambda x^{2\kappa}\right] \psi_n(x) = E_n \psi_n(x)
\]  

(A. 1)

Under the scaling transform \(x \rightarrow v = \lambda^{1/[2(\kappa+1)]}x\) we get

\[
\left[-\frac{1}{2}\lambda^{1/(\kappa+1)} \frac{d^2}{dv^2} + \lambda^{1-\kappa/(\kappa+1)} v^{2\kappa}\right] \psi_n^{sc}(v) = E_n \psi_n^{sc}(v)
\]  

(A. 2)

where \(\psi_n^{sc}\) is the scaling transformed wave function of \(\psi_n\). Multiplying both terms of the above equation by \(\lambda^{-1/(\kappa+1)}\) we obtain

\[
\left[-\frac{1}{2} \frac{d^2}{dv^2} + v^{2\kappa}\right] \psi_n^{sc}(v) = \mathcal{E}_n \psi_n^{sc}(v)
\]  

(A. 3)

where

\[
\mathcal{E}_n = \lambda^{-1/(\kappa+1)}E_n
\]  

(A. 4)
Obviously, the eigenfunctions $\psi_n^{sc}$ of (A. 3) and their respective eigenvalues $E_n$ are independent of $\lambda$-values. The inverse scaling transform $v \rightarrow x = \lambda^{-1/[2(\kappa+1)]}v$ lead to

$$\psi_n(x) = \alpha \psi_n^{sc}(\lambda^{1/[2(\kappa+1)]}x) ,$$

(A. 5)

with $\alpha$ obtained requesting that both, the origin and the scaling transformed one, are normalized to unit,

$$\int \psi_n^2(x) dx = \alpha^2 \int \left[\psi_n^{sc}(\lambda^{1/[2(\kappa+1)]}x)\right]^2 dx = \alpha^2 \lambda^{-1/[2(\kappa+1)]} \int \left[\psi_n^{sc}(v)\right]^2 dv$$

then

$$\int_{-\infty}^{\infty} \psi_n^2(x) dx = \int_{-\infty}^{\infty} \left[\psi_n^{sc}(v)\right]^2 dv = 1 \quad \rightarrow \quad \alpha = \lambda^{1/[4(\kappa+1)]} .$$

(A. 6)

Hence, the relation between the original and the scaling transform eigenfunctions (A. 3) is given by

$$\psi_n(x) = \lambda^{1/[4(\kappa+1)]} \psi_n^{sc}(\lambda^{1/[2(\kappa+1)]}x) ,$$

(A. 7)

with the corresponding relation between the energy eigenvalues (A. 4),

$$E_n = \lambda^{1/(\kappa+1)}E_n$$

(A. 8)

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