Alternative approach to solve the 1-D quantum harmonic oscillator



J. García Ravelo¹, A. L. Trujillo¹, A. Queijeiro¹, J. J. Peña²

¹Departmento de Física, Escuela superior de Física y Matemáticas, Instituto Politécnico Nacional, Edificio 9, U. P. Adolfo López Mateos, CP 07738, México, D. F. ²Univesidad Autonoma Metropolitana - Azcapotzalco, CBI - Área de Física Atómica Molecular Aplicada, Av. San Pablo 180, CP 02200, México, D. F.

E-mail: alto0203@lycos.com

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Abstract

In standard courses of Quantum Mechanics the harmonic oscillator is frequently resolved through of different techniques. In this paper, we introduce another didactic method to obtain its energy spectrum and wave functions by using directly the Hermite polynomials. To do this we only use arguments of general soundness.

Keywords: Harmonic oscillator, Schrödinger equation, Hermite polynomials.

Resumen

En cursos normales de Mecánica Cuántica, el oscilador armónico es frecuentemente resuelto a través de diferentes técnicas. En este artículo, introducimos otro método didáctico para determinar su espectro de energía y sus funciones de onda, usando directamente polinomios de Hermite. Para hacer esto solamente consideramos argumentos de validez general.

Palabras clave: Oscilador armónico, ecuación de Schrödinger, polinomios de Hermite.

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I. INTRODUCTION

The harmonic oscillator potential has been extensively applied in the study of several systems of Theoretical Physics [1]. Besides this potential admits a variety of methods of solution, which is extremely attractive in the courses of Quantum Mechanics. In particular, the 1-D harmonic oscillator can be typically resolved by power series or algebraically through an operator method [2] which can be generalized with the help of supersymmetry and the concept of shape-invariant potentials [3]. Recently, a Fourier transform approach to the system was proposed in order to obtain its solution [4]. In this paper, we show how the 1-D harmonic oscillator can be solved from a different approach improving some general consequences of the Schrödinger equation and properties of the Hermite polynomials, which has not been considered in standard techniques [2, 3, 4, 5]. For this reason we think this method may be opportune in the teaching of Quantum Mechanics.

II. METHOD

We are interested in those potentials of the Schrödinger equation

$$\frac{d^2 \Psi_n}{dx^2} = -\frac{p_n^2}{\hbar^2} \Psi_n; \ p_n^2 = 2m \big(E_n - V(x) \big), \qquad (1)$$

that admit ansatz solution of the form

$$\Psi_n(x) = \boldsymbol{\ell}^{-\xi(x)} \boldsymbol{\upsilon}_n(x), \qquad (2)$$

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where $\xi(x)$ is a real function and

$$\upsilon_n(x) \equiv \sum_{j=0}^n a_{nj} f_j(x); \quad n = 0, 1, 2, 3, ...,$$
(3)

with $f_j(x)$ a polynomial of degree *j*, which can be identified with any element of a basis of polynomials. In fact, the *n* nodes of the wave function $\Psi_n(x)$ are determined by the polynomial $\upsilon_n(x)$. Here, we note that for these solutions, the function $\xi'(x)$ is the logarithm derivative of the ground state $\Psi_0(x)$. Making use of Eq. (2) in Eq. (1) we get the differential equation

$$[(\xi'(x))^2 - \xi''(x)]\nu_n(x) - 2\xi'(x)\nu'_n(x);$$

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$$+\upsilon_{n}^{"}(x) = -\frac{p_{n}^{2}}{\hbar^{2}}\upsilon_{n}(x), \qquad (4)$$

or, using the definition for p_n^2 in Eq. (1),

$$\left[(\xi'(x))^2 - \xi''(x) + \frac{2m}{\hbar^2} (E_n - V(x)) \right] \upsilon_n(x) - 2\xi'(x) \upsilon_n'(x) + \upsilon_n''(x) = 0, \quad n = 0, 1, 2, 3, \dots$$
(5)

Since $\Psi_0(x) \neq 0$, it is easy to see that Eq. (3) and Eq. (5), for n = 0, imply

$$\Psi_0(x) = a_{00} e^{-\xi(x)},$$
 (6)

$$V(x) = \frac{\hbar^2}{2m} \left[\left(\xi'(x) \right)^2 - \xi''(x) \right] + E_0.$$
 (7)

Then the function $\xi(x)$ is linked to the potential V(x) by means of the Riccati equation (7) which is familiar in the development of Supersymmetric Quantum Mechanics (SUSYQM), where $\xi'(x)$ is generally called the *superpotential* of the problem [6]. Other few special cases of Eq. (5) are obtained when n = 1, 2, 3, ...

$$\frac{2m}{\hbar^2} (E_1 - E_0) (a_{10}f_0 + a_{11}f_1(x)) -2\xi'(x)a_{11}f_1'(x) = 0, \qquad (8)$$

$$\frac{2m}{\hbar^{2}} (E_{2} - E_{0}) (a_{20}f_{0} + a_{21}f_{1}(x) + a_{22}f_{2}(x))$$

$$-2\xi'(x) (a_{21}f_{1}(x) + a_{22}f_{2}(x)) + a_{22}f_{2}'(x) = 0,$$
(9)
$$\frac{2m}{\hbar^{2}} (E_{3} - E_{0})$$

$$(a_{30}f_{0} + a_{31}f_{1}(x) + a_{32}f_{2}(x) + a_{33}f_{3}(x))$$

$$-2\xi'(x) (a_{31}f_{1}(x) + a_{32}f_{2}(x) + a_{33}f_{3}(x))$$

$$+a_{32}f_{2}''(x) + a_{33}f_{3}''(x) = 0,...$$
(10)

In particular, if we consider that the function $\xi(x)$ is a polynomial of degree p+1, then V(x) is a polynomial of degree 2p, and Eq. (7) can be arranged as a linear combination of elements of the basis $\{f_j(x)\}_{j=0}^{\infty}$, whose sum is equal to zero. Consequently each coefficient of such

combination must be zero [7]. So, Eq. (7) represents an equation system, from which, E_0 can be obtained. By an analogous argument, the coefficients a_{10} , a_{11} (a_{20}, a_{21}, a_{22}) and the eigenvalue E_1 (E_2) are given via Eq. (8) (Eq. (9))..., here some consequences of Schrödinger equation have to be used. This last point will be explicitly explained below. In general, we can note that the eigenvalue E_n and the coefficients a_{nj} (j = 0,1,2,...n; n = 1,2,3,...) are obtained from Eq. (5) and are independent of the coefficients $a_{n'k}$, (k = 0,1,2,...n') for $n \neq n'$. The particular case when p=1 and $f_j(x)$ is the canonical basis

 x^{j} reproduces the standard solution for the quantum onedimensional harmonic oscillator [8]. Now, in this paper we elect $f_{j}(x) = H_{j}(x)$, with $H_{j}(x)$ the *j*-degree Hermite polynomial.

We propose in Eq. (7) the potential

$$V(x) = AH_{2}(x) + BH_{1}(x).$$
(11)

If we solve the equation

$$V'(x) = AH'_{2}(x) + BH'_{1}(x) = 0,$$
 (12)

by using $H'_{n}(x) = 2nH_{n-1}(x)$ [9] we get

$$H_1(x) = -(B/2A)H_0(x).$$
(13)

Then, substituting Eq. (13) in Eq. (11) we obtain the minimum value of the potential

$$V_{min} = -B^2 / 4A - 2A, \qquad (14)$$

Furthermore, since V_{min} is the minimum value of the potential and V''(x) = 8A, then A > 0. Eqs. (7) and (11) suggest us to write.

$$\xi(x) = \sum_{k=0}^{2} \beta_{k} H_{k}(x), \qquad (15)$$

which implies that

$$\beta_1 = \pm \frac{1}{\hbar} \left(\frac{m}{8}\right)^{1/2} \frac{B}{A^{1/2}}, \ \beta_2 = \pm \frac{1}{\hbar} \left(\frac{m}{8}\right)^{1/2} A^{1/2}, \quad (16)$$

and

$$E_0 = -2\frac{\hbar^2}{m}(\beta_1^2 + 8\beta_2^2 - 2\beta_2), \qquad (17)$$

where the identities

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$$H_0^2(x) = H_0(x) = 1, \ H_2(x) = H_1^2(x) - 2H_0(x), \ (18)$$

were used. Also, by Eqs. (14) and (16), Eq. (17) can be written as

$$E_0 = V_{min} \pm \hbar \left(\frac{2A}{m}\right)^{1/2}.$$
 (19)

The minus sign in this equation needs to be discarded consistently with the well-known proposition *E* must exceed the minimum value of V(x) [10], then the sign for the coefficients β_1 and β_2 in Eq. (16) must be positive, and Eq. (6) gives

$$\Psi_0(x) = a_{00} e^{-\frac{2}{\sum_{k=0}^{\infty} \beta_k H_k(x)}}.$$
 (20)

Therefore, the ground state and its energy eigenvalue are simultaneously obtained. In words, the parameters β_i , i = 1,2 are attained from the equation system generated by Eq. (7), and the sign of β_i is determined from the properties of the Schrödinger equation. Next, the coefficients a_{00} and β_0 are fixed by normalization of $\Psi_0(x)$.

Now, from Eq. (15) and Eq. (17) we substitute $\xi'(x)$ and E_0 in Eq. (8) and obtain.

$$\frac{2m}{\hbar^2} (E_1 - E_0) a_{10} - 8\beta_1 a_{11} + H_1(x) \left(\frac{2m}{\hbar^2} (E_1 - E_0) - 16\beta_2\right) a_{11} = 0. \quad (21)$$

Since $a_{11} \neq 0$, this equation implies

$$E_1 = E_0 + 8\frac{\hbar^2}{m}\beta_2 = -2\frac{\hbar^2}{m}(\beta_1^2 + 8\beta_2^2 - 6\beta_2), \quad (22)$$

and

$$a_{10} = \frac{4\beta_1 \hbar^2}{m(E_1 - E_0)} a_{11} = \frac{\beta_1}{2\beta_2} a_{11} \equiv \frac{B}{2A} a_{11}.$$
 (23)

Then, the first excited state can be written as

$$\Psi_{1}(x) = \left(\frac{B}{2A} + H_{1}(x)\right) a_{11} e^{-\frac{2}{\lambda} - \beta_{\lambda} H_{\lambda}(x)}, \quad (24)$$

here the coefficient a_{11} and the parameter β_0 normalize $\Psi_1(x)$. We note, that Eq. (21) generates two Alternative approach to solve the 1-D quantum harmonic oscillator conditions which allow us to know the parameters a_{10} and E_1 .

Now, when Eq. (9) is considered we have

$$\frac{2m}{\hbar^2} (E_2 - E_0) a_{20} - 8\beta_1 a_{21} + 8(1 + 8\beta_2) a_{22}$$

+ $H_1(x) \left[\left(\frac{2m}{\hbar^2} (E_2 - E_0) - 16\beta_2 \right) a_{21} - 16\beta_1 a_{22} \right]$
+ $H_2(x) \left[\frac{2m}{\hbar^2} (E_2 - E_0) - 32\beta_2 \right] a_{22} = 0, \quad (25)$

then

$$E_2 = E_0 + 16\frac{\hbar^2}{m}\beta_2 = -2\frac{\hbar^2}{m}(\beta_1^2 + 8\beta_2^2 - 10\beta_2), (26)$$

also

$$\left(\frac{2m}{\hbar^2} 16\frac{\hbar^2}{m}\beta_2 - 16\beta_2\right) a_{21} = 16\beta_1 a_{22}, \qquad (27)$$

or

$$a_{21} = \frac{\beta_1}{\beta_2} a_{22} \equiv \frac{B}{A} a_{22}.$$
 (28)

Finally

so

$$\frac{2m}{\hbar^2} 16 \frac{\hbar^2}{m} \beta_2 a_{20} = 8 \frac{\beta_1^2}{\beta_2} a_{22} - 8(1 + 8\beta_2) a_{22},$$

$$a_{20} = \left(\left(\frac{\beta_1}{2\beta_2} \right)^2 - \frac{1}{4\beta_2} + 2 \right) a_{22}.$$
 (29)

Therefore

$$\Psi_{2}(x) = \left[\left(\frac{\beta_{1}}{2\beta_{2}} \right)^{2} - \frac{1}{4\beta_{2}} + 2 + \frac{B}{A} H_{1}(x) + H_{2}(x) \right] a_{22} e^{-\sum_{k=0}^{2} \beta_{k} H_{k}(x)}.$$
(30)

We can continue this process to obtain another quantum states and its eigenvalues in terms of the coefficients of the potential given in (11).

III. PARTICULAR CASE

These results are consistent with those obtained when we take the particular values $A = \frac{1}{8}m\omega^2$ and B = 0, for the shifted zero-point quantum harmonic oscillator.

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The above expressions (19), (20), (22), (24), (26) and (30) reduce to

$$E_0 = \frac{1}{2}\hbar\omega + V_{min}^{AB}, \qquad (31)$$

$$\Psi_0(x) = a_{00} H_0(x) e^{-\frac{m\omega}{2\hbar}x^2},$$
(32)

$$E_1 = \frac{3}{2}\hbar\omega + V_{min}^{AB}, \qquad (33)$$

$$\Psi_1(x) = a_{11} \alpha^{1/2} H_1(x) e^{-\frac{m\omega}{2\hbar}x^2},$$
 (34)

$$E_2 = \frac{5}{2}\hbar\omega + V_{min}^{AB}, \qquad (35)$$

$$\Psi_{2}(x) = a_{22} \left(\alpha H_{2}(x) + 2\alpha - 2 \right) e^{-\frac{m\omega}{2\hbar}x^{2}}, \quad (36)$$

where $V_{min}^{AB} = -m\omega^2/4$, $\alpha = m\omega/\hbar$, $\beta_0 = \alpha/4$ and redefined $a_{nn} \rightarrow a_{nn}/(\alpha^{1/2})^n$. In general, making $x \rightarrow x\alpha^{1/2}$ in (32), (34) and (36), the functions $\Psi_n(x)$ are identified with the standard result [2].

The following possibility, is the called anharmonic oscillator given by $V(x) = Dx^4 + Fx^3 + Ax^2 + Bx$, in this case, the method produces trivial solutions and the corresponding $\Psi_0(x)$ is a non-normalizable function. In fact, this potential does not admit solutions of the form (2).

IV. CONCLUSION

We have presented an alternative didactic method that allows us to resolve the quantum *1-D* harmonic oscillator. This method can be used in standard courses of Quantum Mechanics, since it systematically requires some mathematical properties of the Schrödinger equation and of the Hermite polynomials, and can be used to introduce some basic aspects of SUSY QM.

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