

Hermitian operators and boundary conditions

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The case of the hermiticity of the operators representing the physical observable has received considerable attention in recent years. In this paper we work with a method developed by Morsy and Ata [1] for obtaining Hermitian differential operators independently of the values of the boundary conditions on wave functions. Once obtained these operators, called intrinsically Hermitic operators, we build the Hamiltonian for the harmonic oscillator, hydrogen atom and the potential well of infinite walls. In the first two cases we use the factorization method of ladder operators (also intrinsically Hermitic) and show that results obtained with conventional operators, based on the annulation of the wave functions on the boundaries, are preserved. For the infinite well we show that the version of the Hamiltonian intrinsically Hermitic provides a solution to a paradox that appears in a particular wave function.

Keywords: Boundary conditions; Dirac delta function.

El caso de la hermiticidad de los operadores que representan a los observables ha recibido una atención considerable en los últimos años. En este trabajo tratamos con un método desarrollado por Morsy y Ata [1] para obtener operadores diferenciales hermiticos independientemente de los valores en la frontera que se impongan sobre las funciones de onda. Una vez obtenidos estos operadores, llamados intrínsecamente hermíticos, construimos hamiltonianos para el oscilador armónico, el átomo de hidrógeno y el pozo de potencial de paredes infinitas. En los dos primeros casos utilizamos el método de factorización con operadores de escalera (también intrínsecamente hermíticos) y mostramos que se preservan los resultados obtenidos con los operadores convencionales que se basan en la anulación de las funciones de onda en las fronteras. En el caso del pozo infinito mostramos que la versión intrínsecamente hermítica del hamiltoniano proporciona una solución a una paradoja que se presenta en una función de onda particular.

Descriptores: Condiciones de frontera no nulas.

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1. Introduction

The question of the nature of the eigenvalues of operators in quantum mechanics is fundamental for the correct interpretation of the Schrödinger equation, which along with the boundary conditions, provides all the information we can get about a quantum system. Hermitian operators are traditionally used because their eigenvalues are real numbers which are associated with the values that physical variables take, because have been postulated that these quantities appear in the nature, *i.e.*, they can be measured. For this reason, the physical variables must be associated to operators with suitable properties, but it is important to note that eigenvalues and eigenfunctions depend also of the boundary conditions and for that reason these boundary conditions must be treated with the same care. For differential operators, as the momentum and kinetic energy, this is done in a special way. In fact, in order to the differential operators satisfy the hermiticity notion in the algebraic sense, which is the more accepted, the wave functions must be null on the boundary. For example, bound systems satisfy this almost automatically. However, as in [2] has been indicated for the potential well of infinite walls, some inconsistencies appear from de question if the Hamiltonian of the free particle

$$\hat{H} = -\frac{1}{2} \frac{d^2}{dx^2}$$

is Hermitian. Inconsistencies found in that paper are related to $\langle E \rangle$ and $\langle E^2 \rangle$ where E represents the energy, which arise precisely of the behavior of certain solutions of the Schrödinger equation $\hat{H}\Psi = E\Psi$ on the boundaries of the infinite well.

Just to highlight the interest that exists on the topic of Hermiticity, we should mention that in the literature are other approaches. For example, Ref. 3 treat with respect the Hermitian quantum mechanics in the traditional form, *i.e.*, usual definition of the Hermitian operator and the scalar product in terms of an integral whose limits are the physical boundaries of the system (as we shall see in the next section) is used. The authors propose to eliminate both notions and develop a method that respects the following conditions: the real eigenvalues of an operator representing an observable, the unitarity of the temporal evolution and the correct probabilistic interpretation. These three conditions are essential [4]. They introduce a new notion of Hermiticity based on PT symmetry, parity and temporal inversion and considering the three fundamental conditions. This line of research has generated a considerable production, and some researchers believe that this approach is equivalent to ordinary quantum mechanics but based on a different scalar product [5], while others consider it as an extension of quantum theory [6]. Another interesting way to treat the mathematical nature of the Hamiltonian is a variant of the previous approach, presented in Ref. 7.

A third approach that receives constant attention in the literature is the Dirac algebraic factorization [8] of the Hamiltonian operator for certain systems like the harmonic oscillator, which has been extended to families of potentials with algebras based on Ricatti's parameters that lead to the same energy spectrum of the harmonic oscillator [9]. Versions of these families for supersymmetric quantum mechanics [10] has been developed. Factorization may have aspects which have not been explored extensively. Some mathematical foundations are found in references [11,12] and in the extension to supersymmetric quantum mechanics with Riccati's parameters in Ref. 13.

In this paper we keep the scheme with respect to the Hermitian Dirac operator \hat{A} , *i.e.*, $\hat{A} = \hat{A}^\dagger$, with the ordinary scalar product, but with the novelty that it is not necessary that wave functions be null on the boundaries. This scheme was introduced by Morsy and Ata (MA) in Ref. 1 and is based on the terms with the boundary conditions are absorbed in a new operator \hat{A} which is intrinsically Hermitic, *i.e.*, $\hat{A} = \hat{A}^\dagger$, independently of the values of the wave functions on the boundaries. This new operator must satisfies, of course, the three basic postulated. In this paper a generalization of the MA method is presented which is based on factorization of the intrinsically Hermitic operator \hat{H} and showing that the sets of eigenvalues and eigenfunctions of \hat{H} are exactly the same as the conventional operator \hat{H} for well-known cases of the harmonic oscillator and hydrogen atom. Also give an adequate solution to the paradoxes [2] presented in the well of infinite walls.

This paper is organized as follows: In Sec. 2, Hermitian operators of momentum and kinetic energy in the conventional form and its dependence on boundary conditions are presented along with the concept of intrinsic Hermiticity according to the MA method. In Sec. 3 the new Hamiltonian for the harmonic oscillator is constructed and factored into the ladder operators for showing that the energy spectrum and the set of wave functions are not altered. In Sec. 4 we do the same for the hydrogen atom with ladder operators that change the angular momentum for each energy level in the same way that traditional operators, and also construct the corresponding set of solutions. In Sec. 5 we discuss the consequences that occur in the particular case of a wave function for the potential well of infinite walls that does not vanish at these walls. Section 6 presents the conclusions and finally, in Appendix we developed a formal concept of the Dirac's delta, which justifies the generalization of the MA method to the case where the boundaries go to infinity and the question of the normalization of wave functions.

2. Intrinsic Hermiticity

2.1. Definition

Let $|f\rangle$ and $|g\rangle$ vectors of a vector space with arbitrary scalar product. The above are, in general terms, vectors that are superposition of the elements of some basis. If \hat{A} is a linear

operator, its adjoint \hat{A}^\dagger (if there exists) is defined in the following form:

$$\langle f | \hat{A} | g \rangle = \langle g | \hat{A}^\dagger | f \rangle^* \tag{2.1}$$

If

$$\hat{A}^\dagger = \hat{A} \tag{2.2}$$

i.e., if for all $|f\rangle$ we have

$$\hat{A}^\dagger |f\rangle = \hat{A} |f\rangle$$

then \hat{A} is called Hermitian or self-adjoint operator. In this case Equation (2.1) is now

$$\langle f | \hat{A} | g \rangle = \langle g | \hat{A} | f \rangle^* \tag{2.3}$$

Note that the Hermiticity condition (2.2) is independent of the vector space considered, the basis used and therefore any particular representation. Taking into account and in accordance with Morsy and Ata, the condition (2.2) expresses the named intrinsic Hermiticity of the operator \hat{A} which, in terms of the scalar product, is given by (2.3). We apply this to the Hilbert space of solutions of the Schrödinger equation. With the scalar product defined in the usual way

$$\langle f | \hat{A} | g \rangle = \int_{x_1}^{x_2} f^*(x) \hat{A}g(x) dx$$

Eq. (2.3) is now

$$\int_{x_1}^{x_2} f^*(x) \hat{A}g(x) dx = \left[\int_{x_1}^{x_2} g^*(x) \hat{A}f(x) dx \right]^* \tag{2.4}$$

which is the definition of Hermitian operator in quantum mechanics [4]. As is well-known, it is necessary to impose an extra condition when \hat{A} is the differential operator

$$\vec{D} = \frac{d}{dx}$$

or a polynomial function of \vec{D} (the arrow on the letter D acquires a precise meaning later.) In effect:

$$\begin{aligned} \langle f | \frac{d}{dx} | g \rangle &= \int_{x_1}^{x_2} f^*(x) \frac{d}{dx} g(x) dx \\ &= f^*(x) g(x) \Big|_{x_1}^{x_2} - \langle g | \frac{d}{dx} | f \rangle^* \end{aligned} \tag{2.5}$$

The extra condition consider that the functions must be null on the boundaries. However this is not enough; even in this case, the derivative operator is not Hermitian, *i.e.*, does not satisfy (2.4), due to the sign of the second term of (2.5).

For the second derivative we have two extra terms because we have two integrations

$$\langle f | \frac{d^2}{dx^2} | g \rangle = f^*(x) \frac{d}{dx} g(x) \Big|_{x_1}^{x_2} - g(x) \frac{d}{dx} f^*(x) \Big|_{x_1}^{x_2} + \langle g | \frac{d^2}{dx^2} | f \rangle^* \quad (2.6)$$

In the simplest quantum case we have the momentum operator

$$\hat{p} = -i \frac{d}{dx}$$

for which

$$\begin{aligned} \langle f | \hat{p} | g \rangle &= \int_{x_1}^{x_2} f^*(x) \hat{p} g(x) dx \\ &= -i f^*(x) g(x) \Big|_{x_1}^{x_2} + \langle g | \hat{p} | f \rangle^* \end{aligned} \quad (2.7)$$

Unless the wave functions be null on the boundaries x_1 and x_2 , the momentum operator is not intrinsically Hermitic in the sense of Eq. (2.2) or (2.3) for differential operators. For the kinetic energy operator

$$\hat{T} = -\frac{1}{2} \frac{d^2}{dx^2}$$

we have, according to (2.6)

$$\begin{aligned} \langle f | \hat{T} | g \rangle &= -\frac{1}{2} f^*(x) \frac{d}{dx} g(x) \Big|_{x_1}^{x_2} \\ &+ \frac{1}{2} g(x) \frac{d}{dx} f^*(x) \Big|_{x_1}^{x_2} + \langle g | \hat{T} | f \rangle^* \end{aligned} \quad (2.8)$$

As a consequence of (2.8) the Hamiltonian of the quantum system is considered only Hermitic when the wave functions and/or its derivatives are null on the boundaries. For bound systems this happens almost always, but other type of problems, for example, dispersion problems, the functions are not null on the boundary. As a curious note, in Ref. 2 the authors discuss some paradoxes about the Hermiticity of the Hamiltonian relative to the values that certain wave function of a particle in an infinite potential well takes, and then provide an explanation. As mentioned, the method presented in this paper provides a natural solution to this situation.

2.2. Method of hermitization

Here we present the mechanism developed in Ref. 1 by Morsy and Ata (MA method) in which the boundary conditions are not used in the conventional role. In this mechanism the boundary terms of (2.7) and (2.8) are absorbed into new operators of momentum and kinetic energy and the same technique is used for any linear combination of differential operators.

We introduce the extended Dirac delta

$$\tilde{\delta} = \delta(x, x_1, x_2) = \delta(x - x_2) - \delta(x - x_1) \quad (2.9)$$

with which we can write a function evaluated in the points x_1 and x_2 in the form

$$\begin{aligned} F(x) \Big|_{x_1}^{x_2} &= F(x_2) - F(x_1) = \int_{x_1}^{x_2} F(x) \delta(x - x_2) dx \\ &- \int_{x_1}^{x_2} F(x) \delta(x - x_1) dx = \int_{x_1}^{x_2} F(x) \tilde{\delta} dx \end{aligned} \quad (2.10)$$

Using (2.10) we can write the boundary terms of (2.5) in the form

$$f^*(x) g(x) \Big|_{x_1}^{x_2} = \int_{x_1}^{x_2} f^*(x) g(x) \tilde{\delta} dx = \langle g | \tilde{\delta} | f \rangle^*$$

and substituting in (2.5) we find

$$\langle f | \vec{D} | g \rangle = \langle g | \tilde{\delta} | f \rangle^* - \langle g | \vec{D} | f \rangle^* = \langle g | (\tilde{\delta} - \vec{D}) | f \rangle^*$$

Then we can write the adjoint of \vec{D} as [1]

$$\vec{D}^\dagger = \tilde{\delta} - \vec{D} \quad (2.11)$$

For the second derivative we obtain from (2.6)

$$\begin{aligned} \langle f | \vec{D}^2 | g \rangle &= \langle g | \overleftarrow{D} \tilde{\delta} | f \rangle^* - \langle g | \tilde{\delta} \vec{D} | f \rangle^* + \langle g | \vec{D}^2 | f \rangle^* \\ &= \langle g | (\overleftarrow{D} \tilde{\delta} - \tilde{\delta} \vec{D} + \vec{D}^2) | f \rangle^* \\ \vec{D}^{2\dagger} &= \overleftarrow{D} \tilde{\delta} - \tilde{\delta} \vec{D} + \vec{D}^2 \end{aligned} \quad (2.12)$$

where the following symbology has been introduced

$$\vec{D} | f \rangle \rightarrow \frac{d}{dx} f(x), \quad \langle f | \overleftarrow{D} \rightarrow f(x) \frac{d}{dx}$$

to continue using the Dirac notation in a coherent way.

With the mechanism of the extended Dirac delta the expression (2.5), along with the factor $-i$ used for the moment operator, takes the form:

$$\langle f | \hat{p} | g \rangle = \langle g | (i\tilde{\delta} - \hat{p}) | f \rangle^* \quad (2.13)$$

Using (2.13) and (2.1), which defines the adjoint operator, we obtain the adjoint of the momentum operator

$$\hat{p}^\dagger = i\tilde{\delta} - i \frac{d}{dx} = i\tilde{\delta} + \hat{p} \quad (2.14)$$

Making the same with the operator of kinetic energy we obtain

$$\hat{T}^\dagger = -\overleftarrow{D} \tilde{\delta} \frac{1}{2} + \frac{1}{2} \tilde{\delta} \vec{D} + \hat{T} \quad (2.15)$$

The MA method take the individual operators that appear in the adjoint and make a linear combination of them with coefficients chosen adequately in order to obtain hermiticity of that linear combination which is called associate differential

operator (ADO). For derivative operator (2.11) the ADO is given by

$$\vec{D} = a_0 \tilde{\delta} + a_1 \vec{D}$$

which must be equal to its adjoint:

$$\begin{aligned} \vec{D}^\dagger &= a_0^* \tilde{\delta} + a_1^* \vec{D}^\dagger \\ &= a_0^* \tilde{\delta} + a_1^* (\tilde{\delta} - \vec{D}) = (a_0^* + a_1^*) \tilde{\delta} - a_1^* \vec{D} \end{aligned}$$

from where $a_1 = -a_1^*$, $a_0 = a_0^* + a_1^*$. From these relations we obtain $a_1 = i$ and $a_0 - a_0^* = -i = 2Im a_0$, i.e., $a_0 = \tilde{\alpha} - i/2$, where $\tilde{\alpha}$ is a real number. Then the intrinsically Hermitic derivative operator is:

$$\vec{D} = i\vec{D} + \left(\tilde{\alpha} - \frac{i}{2}\right) \tilde{\delta} = i\vec{D} - c(x) = -\hat{p} - c(x) \quad (2.16)$$

where

$$c(x) = \left(-\tilde{\alpha} + \frac{i}{2}\right) \tilde{\delta} \quad (2.17)$$

Taking into account the operators appearing in (2.12), the ADO of the second derivative is:

$$\vec{D}^2 = b_0 \overleftarrow{D} \tilde{\delta} + b_1 \tilde{\delta} \overrightarrow{D} + b_2 \vec{D}^2 \quad (2.18)$$

which must be equal to its adjoint. From this $b_0 = b_1^* + b_2^*$ and $b_2 = b_2^* = 1$ and thus b_0 or b_1 are indeterminate. If we choose $b_0 = \beta$ then $b_1 = \beta^* - 1$ and the operator for the second derivative is:

$$\vec{D}^2 = \vec{D}^2 + \overleftarrow{D} \tilde{\delta} \beta + (\beta^* - 1) \tilde{\delta} \overrightarrow{D} \quad (2.19)$$

Using (2.16) and (2.19) we can write the momentum and kinetic energy operators intrinsically Hermitic in the following form

$$\hat{p} = -\vec{D} = \hat{p} + c(x) \quad (2.20)$$

$$\hat{T} = -\frac{1}{2} \vec{D}^2 = -\frac{1}{2} \left[\vec{D}^2 + \overleftarrow{D} \tilde{\delta} \beta + (\beta^* - 1) \tilde{\delta} \overrightarrow{D} \right] \quad (2.21)$$

The Hamiltonian \hat{H} of a quantum system that is subject to a potential $V(x)$, is

$$\hat{H} = \hat{T} + V(x) = \frac{1}{2} \hat{p}^2 + V(x) \quad (2.22)$$

and also is intrinsically Hermitic. In the case of the fourth derivative, which we will use in Sec. 5 for the infinite well, we obtain:

$$\begin{aligned} \vec{D}^4 &= c_0 \overleftarrow{D}^3 \tilde{\delta} + c_1 \overleftarrow{D}^2 \tilde{\delta} \overrightarrow{D} \\ &+ c_2 \tilde{\delta} \overrightarrow{D}^2 + c_3 \tilde{\delta} \overrightarrow{D}^3 + c_4 \vec{D}^4 \end{aligned} \quad (2.23)$$

where the coefficients satisfy $c_4 = 1$, $c_0 + c_3 = \gamma$, $c_1 + c_2 = \eta$, with γ and η real numbers.

We summarize the mechanism of the MA method for any linear differential operator \hat{A} as follows: a) evaluate the adjoint of \hat{A} using integration by parts taking terms of the

boundary as part of the adjoint and identifying the individual operators involved as a basis; b) define the ADO of \hat{A} by a linear combination of this basis, with complex coefficients, c) determine the adjoint \hat{A}^\dagger of the ADO and d) match the two operators $\hat{A} = \hat{A}^\dagger$ for obtaining a set of algebraic equations for the coefficients. Taking into account that some coefficients are undetermined, we have an infinite set of intrinsically Hermitic versions of \hat{A} . Additional information is required from each quantum system to determine in unique form all coefficients.

In the Appendix is demonstrated another contribution to the MA method which is the extension to the case of the hydrogen atom and harmonic oscillator when the boundaries extend to infinity.

2.3. Commutation Relationship between \hat{p} and \hat{x}

We start from the conventional commutator

$$[\hat{x}, \hat{p}] = [\hat{x}, -i\vec{D}] = i \quad (2.24)$$

to evaluate the comutator of the intrinsically Hermitic momentum operator \hat{p} and the position operator \hat{x} .

$$[\hat{x}, \hat{p}] = \left[\hat{x}, \hat{p} - \left(\alpha - \frac{i}{2}\right) \tilde{\delta} \right] = [\hat{x}, \hat{p}] - \left(\alpha - \frac{i}{2}\right) [\hat{x}, \tilde{\delta}]$$

Using expression (2.9) for the extended Dirac delta, we find that $[\hat{x}, \tilde{\delta}] = 0$, since

$$\begin{aligned} \langle f | [\hat{x}, \tilde{\delta}] | g \rangle &= \int_{x_1}^{x_2} f^*(x) \hat{x} \tilde{\delta} g(x) dx \\ &- \int_{x_1}^{x_2} f^*(x) \tilde{\delta} \hat{x} g(x) dx = 0 \end{aligned}$$

which is independent of the values of the functions $f(x)$ and $g(x)$ on the boundary x_1 y x_2 . Then

$$[\hat{x}, \hat{p}] = [\hat{x}, \hat{p}] = i$$

This result is very important because it shows that the intrinsically Hermitic momentum operator satisfies the Heisenberg's uncertainty principle.

3. Harmonic oscillator

In this section intrinsically Hermitic differential operators developed in the previous section are tested in the known case of the harmonic oscillator by the factorization method of Dirac [13].

3.1. Conventional treatment

The harmonic oscillator is one of the most interesting of quantum mechanics which can be solved exactly. The conventional Hamiltonian is given by

$$\hat{H} = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\hat{x}^2 \tag{3.1}$$

where $\hat{p} = -i\vec{D}$. First, we briefly review the algebraic factorization procedure of the Hamiltonian (3.1). With the operators

$$\hat{a} = \frac{i}{\sqrt{2}}\hat{p} + \frac{1}{\sqrt{2}}\hat{x} \tag{3.2}$$

$$\hat{b} = -\frac{i}{\sqrt{2}}\hat{p} + \frac{1}{\sqrt{2}}\hat{x} \tag{3.3}$$

the Hamiltonian can be write

$$\hat{H} = \hat{a}\hat{b} - \frac{1}{2} \tag{3.4}$$

$$\hat{H} = \hat{b}\hat{a} + \frac{1}{2} \tag{3.5}$$

It is easy to find the commutation relation between operators (3.2) and (3.3):

$$[\hat{a}, \hat{b}] = 1 \tag{3.6}$$

and the Schrödinger equation

$$\hat{H}\psi_n = E_n\psi_n \tag{3.7}$$

can be write in the form

$$\hat{H}\psi_n = \left(\hat{a}\hat{b} - \frac{1}{2}\right)\psi_n \tag{3.8}$$

Applying the operator \hat{b} to (3.8) we find the following result

$$\left(\hat{b}\hat{a} + \frac{1}{2}\right)\hat{b}\psi_n = (E_n + 1)\hat{b}\psi_n \tag{3.9}$$

This last expression is equivalent to (3.7). In effect, comparing (3.7) and (3.9) we can see that $\hat{b}\psi_n$ is also a eigenfunction of the Hamiltonian with eigenvalue $E_n + 1$, that is,

$$\hat{H}\hat{b}\psi_n = (E_n + 1)\hat{b}\psi_n$$

so we can say that, except for a proportionality constant, $\hat{b}\psi_n$ represents the state of quantum number $n + 1$:

$$\hat{b}\psi_n \sim \psi_{n+1} \tag{3.10}$$

Therefore \hat{b} is called raising operator. In the same way

$$\hat{a}\psi_n \sim \psi_{n-1} \tag{3.11}$$

from where \hat{a} is a lowering operator. The chain is broken down because the energy can not be negative. Let ψ_0 the minimum energy state or ground state; then $\hat{a}\psi_0 = 0$. The

solution of this differential equation is $\psi_0(x) = e^{-x^2/2}$. Applying the Hamiltonian in the form (3.5) to ψ_0 we find the minimum energy $E_0 = 1/2$. Finally, the state energy

$$E_n = n + \frac{1}{2} \tag{3.12}$$

is obtained applying n times the operator \hat{b} to the ground state:

$$\psi_n \sim \hat{b}^n\psi_0 \sim e^{-x^2/2}H_n(x) \tag{3.13}$$

where $H_n(x)$ the Hermite polynomial of degree n . The expressions (3.12) and (3.13) are the solution for the quantum harmonic oscillator with the conventional Hamiltonian (3.1).

3.2. The intrinsically Hermitian version

We will now use the intrinsically Hermitic version of the Hamiltonian operator applied to the same harmonic oscillator. We make no assumptions about the behavior of the wave functions at the boundaries although is well-known that such functions are null on those boundaries. Our purpose here is to demonstrate that the intrinsic Hermitic Hamiltonian $\hat{\mathbf{H}}$, Eq. (2.22), gives the same results as the conventional Hamiltonian (3.1). We take the Hamiltonian in the form

$$\hat{\mathbf{H}} = \frac{1}{2}\hat{\mathbf{p}}^2 + \frac{1}{2}\hat{x}^2 \tag{3.14}$$

The Schrödinger equation is

$$\hat{\mathbf{H}}\varphi_n = E_n\varphi_n \tag{3.15}$$

in which the energy E_n is the same as in the conventional treatment, but the solution is denoted by $\varphi_n(x)$. Below we will establish the relationship between $\psi_n(x)$ and $\varphi_n(x)$ and show that physics is the same for both solutions. We propose a factorization based in the operators

$$\hat{\mathbf{a}} = \frac{i}{\sqrt{2}}\hat{\mathbf{p}} + \frac{1}{\sqrt{2}}\hat{x} \tag{3.16}$$

$$\hat{\mathbf{b}} = -\frac{i}{\sqrt{2}}\hat{\mathbf{p}} + \frac{1}{\sqrt{2}}\hat{x} \tag{3.17}$$

where $\hat{\mathbf{p}}$ is the intrinsically Hermitic momentum operator (2.20), which also appears in the Hamiltonian (3.14). The new operators have the same functional form as ordinary operators (3.2) and (3.3) and their algebraic properties are the same, for example

$$\hat{\mathbf{a}}\hat{\mathbf{b}} = -\frac{1}{2}\hat{\mathbf{p}}^2 + \frac{1}{2}\hat{x}^2 + \frac{i}{2}[\hat{\mathbf{p}}, \hat{x}] = \hat{\mathbf{H}} + \frac{1}{2}$$

Then we have that the equation (3.15) can be written in the following forms

$$\left(\hat{\mathbf{a}}\hat{\mathbf{b}} - \frac{1}{2}\right)\varphi_n = E_n\varphi_n \tag{3.18}$$

$$\left(\hat{\mathbf{b}}\hat{\mathbf{a}} + \frac{1}{2}\right)\varphi_n = E_n\varphi_n \tag{3.19}$$

$$\left(\hat{\mathbf{a}}\hat{\mathbf{b}} + \hat{\mathbf{b}}\hat{\mathbf{a}}\right)\varphi_n = 2E_n\varphi_n \tag{3.20}$$

with the commutator

$$[\hat{\mathbf{a}}, \hat{\mathbf{b}}] = 1 \tag{3.21}$$

The commutation relation (3.21) shows that the algebra of intrinsically Hermitian operators $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$ is exactly the same as that of the operators \hat{a} and \hat{b} , and from this the energy spectrum is the same as the conventional oscillator, as mentioned before. Now we will generate the wave functions. If φ_0 represents the ground state, then the condition $\hat{\mathbf{a}}\varphi_0 = 0$ allows us find it. In effect, using (2.20) express the operator $\hat{\mathbf{a}}$ in the form (in the coordinate representation):

$$\hat{\mathbf{a}} = \frac{1}{\sqrt{2}} \left[\frac{d}{dx} + ic(x) + x \right]$$

from where we find the differential equation

$$\frac{d\varphi_0}{dx} + [ic(x) + x]\varphi_0 = 0$$

whose solution is

$$\begin{aligned} \varphi_0(x) &\sim e^{-x^2/2} e^{-i \int c(x) dx} \\ &\sim H_0(x) e^{-x^2/2} e^{-i \int c(x) dx} \end{aligned} \tag{3.22}$$

Now, the raising operator

$$\hat{\mathbf{b}} = \frac{1}{\sqrt{2}} \left[-\frac{d}{dx} - ic(x) + x \right] \tag{3.23}$$

generate the first excited state

$$\varphi_1(x) \sim \hat{\mathbf{b}}\varphi_0 \sim H_1(x) e^{-x^2/2} e^{-i \int c(x) dx}$$

where $H_1(x) = 2x$. In general, if

$$\varphi_{n-1}(x) \sim H_{n-1}(x) e^{-x^2/2} e^{-i \int c(x) dx}$$

we get

$$\begin{aligned} \varphi_n(x) &\sim \hat{\mathbf{b}}\varphi_{n-1}(x) \sim [2xH_{n-1}(x) \\ &\quad - H'_{n-1}(x)] e^{-x^2/2} e^{-i \int c(x) dx} \end{aligned}$$

and using the recurrence relation between Hermite polynomials $H'_{n-1} = 2xH_{n-1} - H_n$ we find the expression for the wave function of the n -th excited state

$$\begin{aligned} \varphi_n(x) &\sim H_n(x) e^{-x^2/2} e^{-i \int c(x) dx} \\ &\sim \psi_n(x) e^{-i \int c(x) dx} \end{aligned} \tag{3.24}$$

Finally, as shown in Appendix, we have in the physical interval of the oscillator, *i.e.*, $-\infty < x < \infty$, the additional factor $e^{-i \int c(x) dx} = e$, which contribute to the normalization constant. We have shown that the ladder operators intrinsically Hermitic $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$ generate the same set of eigenfunctions as the conventional operators \hat{a} and \hat{b} . In summary, the factorization of the intrinsically Hermitic Hamiltonian (3.14) is the same as the standard Hamiltonian (3.1), maintaining

the invariability of the oscillator problem: the energy spectrum (3.12) and the collection of wave functions (3.24) with all its properties. Finally, we can say that the intrinsic hermitization of the operators (3.16) and (3.17) according to the MA method, describes in correct form the harmonic oscillator since their algebra is exactly the same as conventional operators (3.2) and (3.3).

4. The hydrogen atom

4.1. Conventional factorization

We consider the radial part of the Schrödinger equation, in which the Coulomb potential $V(r) = -Ze^2/r$ and the energy E_n are. The conventional Hamiltonian

$$\hat{H}_l = -\frac{1}{2r} \frac{d^2}{dr^2} r + \frac{l(l+1)}{2r^2} - \frac{Ze^2}{r} \tag{4.1}$$

such that $\hat{H}_l R_{n,l} = E_n R_{n,l}$ for the principal quantum number n and the quantum number of angular momentum l . To simplify the notation usually the dimensionless variable $\rho = Ze^2 r$, the constant $\lambda = 2E/Z^2 e^4$ and the change $R_{n,l} = \rho \psi_{n,l}$ are introduced. The expression for the Hamiltonian is now

$$\hat{H}_l = -\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2} - \frac{2}{\rho} \tag{4.2}$$

and the Schrödinger equation is now written as $\hat{H}_l \psi_{n,l} = E_n \psi_{n,l}$. The ladder operators are [11]

$$\hat{a}_l = i\hat{p} + \frac{l}{\rho} - \frac{1}{l} \tag{4.3}$$

$$\hat{b}_l = -i\hat{p} + \frac{l}{\rho} - \frac{1}{l} \tag{4.4}$$

with the properties

$$\hat{a}_l \hat{b}_l = \hat{H}_{l-1} + \frac{1}{l^2} \tag{4.5}$$

$$\hat{b}_l \hat{a}_l = \hat{H}_l + \frac{1}{l^2} \tag{4.6}$$

and as a consequence of (4.5) and (4.6) we find the relations

$$\hat{H}_{l-1} \hat{a}_l \psi_{n,l} = \hat{a}_l \hat{H}_l \psi_{n,l} = E_n \hat{a}_l \psi_{n,l} \tag{4.7}$$

$$\hat{H}_{l+1} \hat{b}_l \psi_{n,l} = \hat{b}_l \hat{H}_l \psi_{n,l} = E_n \hat{b}_l \psi_{n,l} \tag{4.8}$$

We have that the functions $\hat{a}_l \psi_{n,l}$ and $\hat{b}_{l+1} \psi_{n,l}$ are eigenfunctions of the Hamiltonian for the values $l-1$ and $l+1$ of the angular moment, respectively, with the same energy E_n and [11]

$$\hat{a}_l \psi_{n,l} \sim \psi_{n,l-1} \tag{4.9}$$

$$\hat{b}_{l+1} \psi_{n,l} \sim \psi_{n,l+1} \tag{4.10}$$

These expressions are analogous to (3.10) and (3.11) of the harmonic oscillator. Algebraic properties (4.5) and (4.6) of ladder operators $\widehat{a}_l, \widehat{b}_l$ determine the structure of angular momentum states. For example, if the quantum number l is defined by the eigenvalue equation $\widehat{L}^2 \psi_{n,l} = l(l+1) \psi_{n,l}$, with \widehat{L}^2 the square of angular momentum, which is a positive definite operator, then $l(l+1) \geq 0$. One consequence is that $l = 0, 1, 2, \dots, n-1$. The raising operator \widehat{b}_l according to the property (4.10), annihilates the state $\psi_{l,l-1}$:

$$\widehat{b}_l \psi_{l,l-1} = 0 \tag{4.11}$$

which is a first order differential equation whose solution is the wave function with the highest value of angular momentum l with energy E_n . The result is

$$\psi_{l,l-1} \sim \rho^l e^{-\rho/l} \tag{4.12}$$

Thus the wave functions for a given n and for all allowed values of l are found [14]:

$$\psi_{n,l} \sim g_{n,l}(\rho) \rho^l e^{-\rho/n} \tag{4.13}$$

4.2. The hydrogen atom with intrinsically Hermitic operators

In this section we solve the same problem of the hydrogen atom considering intrinsically Hermitic operators. We develop the hamiltonian using the kinetic energy and the Coulomb potential. Taking into account (4.2) we propose

$$\widehat{H}_l = -\widehat{p}^2 + \frac{l(l+1)}{\rho^2} - \frac{2}{\rho} \tag{4.14}$$

Using the commutation relations

$$[\rho, \widehat{D}] = [\rho, \widehat{D}_\rho] = [r, \widehat{D}_r] = -1$$

and the ladder operators

$$\widehat{a}_l = i\widehat{p} + \frac{l}{\rho} - \frac{1}{l} \tag{4.15}$$

$$\widehat{b}_l = -i\widehat{p} + \frac{l}{\rho} - \frac{1}{l} \tag{4.16}$$

we obtain the following factorization relations of the Hamiltonian :

$$\widehat{a}_l \widehat{b}_l = \widehat{H}_{l-1} + \frac{1}{l^2} \tag{4.17}$$

$$\widehat{b}_l \widehat{a}_l = \widehat{H}_l + \frac{1}{l^2} \tag{4.18}$$

If $\varphi_{n,l}$ is solution of the Schrödinger equation, with the Hamiltonian (4.16) that is, if

$$\widehat{H}_l \varphi_{n,l} = E_n \varphi_{n,l} \tag{4.19}$$

We can prove that equivalent relations (4.9) and (4.10) are satisfied for the intrinsically Hermitic operators:

$$\widehat{a}_l \varphi_{n,l} \sim \varphi_{n,l-1} \tag{4.20}$$

$$\widehat{b}_{l+1} \varphi_{n,l} \sim \varphi_{n,l+1} \tag{4.21}$$

Particularly, according to (4.11) the solution of the differential equation

$$\widehat{b}_l \varphi_{l,l-1} = 0 \tag{4.22}$$

is given by

$$\varphi_{n,l-1} \sim \rho^l e^{-\rho/n} e^{-i \int c(\rho) d\rho} \tag{4.23}$$

The wave function corresponding to energy E_n are generated using (4.21) and (4.23):

$$\varphi_{n,l} \sim g_{n,l}(\rho) \rho^l e^{-\rho/n} e^{-i \int c(\rho) d\rho} \tag{4.24}$$

In (4.24) the factor $e^{-i \int c(\rho) d\rho} = e$ appears but it has not consequence (as the harmonic oscillator case). Finally, we concluded the factorization method of the hamiltonian (4.14) by the operators (4.17) and (4.18), all of them intrinsically Hermitic, keep the results on of the conventional handle for hydrogen atom.

5. The infinite well of potential

5.1. Conventional handle

In this section we consider the case of the well of potential defined in the following form:

$$V(x) = \begin{cases} 0 & -\frac{L}{2} < x < \frac{L}{2} \\ \infty & |x| \geq \frac{L}{2} \end{cases} \tag{5.1}$$

whose wave functions are of two kinds: the odd

$$\Phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{2n\pi}{L}x\right) \tag{5.2}$$

whose energy spectrum is given by

$$E_n = \frac{1}{2} \left(\frac{2n\pi}{L}\right)^2 \tag{5.3}$$

and the even ones

$$\Psi_n(x) = \sqrt{\frac{2}{L}} \cos\left(\frac{(2n-1)\pi}{L}x\right) \tag{5.4}$$

with

$$E'_n = \frac{1}{2} \left(\frac{(2n-1)\pi}{L}\right)^2 \tag{5.5}$$

Consider the wave function [2]

$$\psi(x) = -\sqrt{\frac{30}{L^5}} \left(x^2 - \frac{L^2}{4}\right) - \frac{L}{2} < x < \frac{L}{2} \tag{5.6}$$

This wave function which satisfies the boundary conditions

$$\psi\left(-\frac{L}{2}\right) = \psi\left(\frac{L}{2}\right) = 0 \tag{5.7}$$

has a series expansion of the complete basis (5.4) of eigenfunctions of the Hamiltonian

$$\hat{H} = -\frac{1}{2}D^2 \tag{5.8}$$

as follows

$$\psi(x) = \sum_{n=1}^{\infty} b_n \Psi_n(x) \tag{5.9}$$

Direct calculation gives us the shape of the coefficients b_n :

$$b_n = \langle \Psi_n | \psi \rangle = \frac{8\sqrt{15}}{\pi^3} \frac{(-1)^{n-1}}{(2n-1)^3} \tag{5.10}$$

Using (2.6) we find that hamiltonian of the free particle:

$$\begin{aligned} \langle \psi | -\frac{d^2}{dx^2} | \psi \rangle &= -\psi^*(x) \frac{d}{dx} \psi(x) \Big|_{-L/2}^{L/2} \\ &- \psi(x) \frac{d}{dx} \psi^*(x) \Big|_{-L/2}^{L/2} + \langle \psi | -\frac{d^2}{dx^2} | \psi \rangle^* \end{aligned} \tag{2.6}$$

However, according to [2] appears an unexpected fact. From (5.10) we find

$$\langle E^2 \rangle = \sum_{n=1}^{\infty} |b_n|^2 (E'_n)^2 = \frac{30}{L^4} \tag{5.11}$$

On the other hand:

$$\begin{aligned} \langle E^2 \rangle &= \langle \psi | \hat{H}^2 | \psi \rangle = \int_{-L/2}^{L/2} \psi^*(x) \hat{H}^2 \psi(x) dx \\ &= \int_{-L/2}^{L/2} \psi^*(x) \hat{H} [\hat{H} \psi(x)] dx = 0 \end{aligned} \tag{5.12}$$

since $\hat{H}\psi(x)$ is a constant:

$$\hat{H}\psi(x) = \sqrt{\frac{30}{L^5}} \tag{5.13}$$

In [2] has been prove that there is not contradiction. In this work we are interested in studying the intrinsic hermiticity of this problem.

5.2. Intrinsically Hermitic Hamiltonian

The MA method is used in this section for studying the same problem of the expectation value $\langle E^2 \rangle$. We consider the Hamiltonian of the free particle, that is (2.21),

$$\hat{H} = -\frac{1}{2}\overrightarrow{D}^2$$

In order to find $\langle E^2 \rangle$ we need the fourth intrinsically Hermitic derivative \overrightarrow{D}^4 , Eq. (2.22):

$$\overrightarrow{D}^4 = c_0 \overleftarrow{D}^3 \overrightarrow{\delta} + c_1 \overleftarrow{D}^2 \overrightarrow{\delta} \overrightarrow{D} + c_2 \overleftarrow{D} \overrightarrow{\delta} \overrightarrow{D}^2 + c_3 \overrightarrow{\delta} \overrightarrow{D}^3 + c_4 \overrightarrow{D}^4$$

It is clear that $\langle \psi | \hat{H}^2 | \psi \rangle \neq 0$ because \overrightarrow{D}^4 has other terms different than \overrightarrow{D}^4 and \overrightarrow{D}^3 , which eliminated to (5.13).

In fact

$$\begin{aligned} \langle E^2 \rangle &= \left(-\frac{1}{2}\right)^2 \langle \psi | \overrightarrow{D}^4 | \psi \rangle \\ &= \left(-\frac{1}{2}\right)^2 \langle \psi | [c_1 \overleftarrow{D}^2 \overrightarrow{\delta} \overrightarrow{D} + c_2 \overleftarrow{D} \overrightarrow{\delta} \overrightarrow{D}^2] | \psi \rangle \end{aligned}$$

Calculating directly we find

$$\langle E^2 \rangle = \frac{1}{4} \left(4\frac{30}{L^5}\right) \eta \int_{-L/2}^{L/2} x \tilde{\delta} dx = \frac{30}{L^4} \eta$$

This result is correct if $\eta = 1$. This is according to comment given at the end of the Sec. 2.2 about the coefficients of the associate differential operator, which is fundamental for hermitization process of the differential operators.

6. Conclusions

In this work the MA mechanism of the intrinsic hermitization has been presented. It produce Hermitic differential operators without the restriction that wave functions be null on the boundaries of the physical system because the boundary terms are absorbed by a new version of the differential operator. This method was originally developed for studying collision problems and has been applied to problems of the mathematical physics. But, in our opinion, the MA method has not explored enough.

The MA method in particular, was applied in two problem which has exact solution: the harmonic oscillator and the hydrogen atom. In both cases the results given by the conventional hamiltonian are preserved when the intrinsically Hermitic Hamiltonian was applied, which is a necessary test: the physics of the boundary conditions. Another application of the MA process, exposed in this work, correspond to the well of infinite walls for calculating the expectation value of the square of the energy, obtaining appropriated results whereas for the conventional hamiltonian contradictories results can be obtained.

We consider for MA method the case when the boundaries go to infinite in order to known if the method is valid in this case. The answer is positive and it is shown in the Appendix. Our final conclusion is: in quantum mechanics there are interesting points which must be manipulated carefully for obtaining correct physical interpretations. We think that MA method can give good results in other applications.

Appendix

A. The extension to infinite

The Dirac delta function $\delta(x)$ can be consider as the limit of bilinear forms $\delta_\alpha(x)$

$$\delta(x) = \lim_{\alpha \rightarrow 0} \delta_\alpha(x) \tag{A.1}$$

Graphics of the bell functions

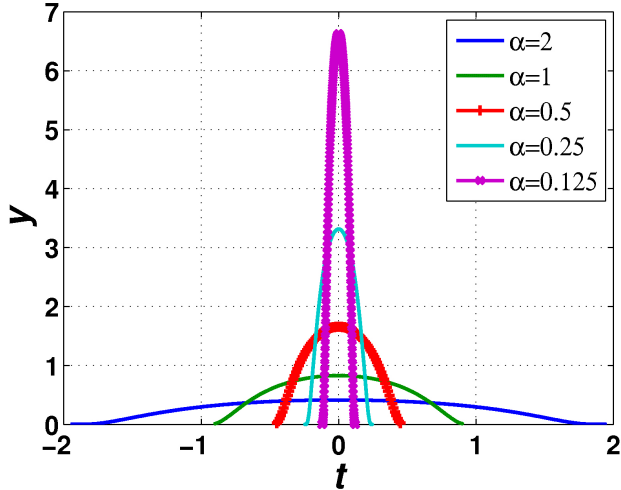


FIGURE 1. Graphics of the bell functions.

Graphics of the semi bell functions

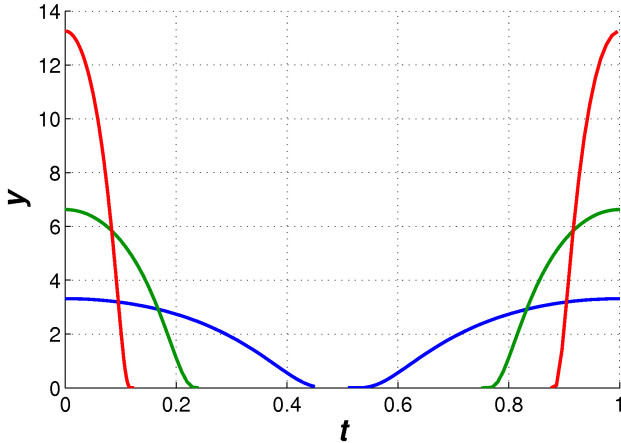


FIGURE 2. Graphics of the semi-bell functions for defining $\tilde{\delta}$.

defined by bell functions centered at $x = 0$:

$$\delta_\alpha(x) = \langle \cdot | g_\alpha(x) | \cdot \rangle : D(\hat{p}) \times D(\hat{p}) \rightarrow C$$

$$\langle f | g_\alpha | g \rangle = \int_{x_1}^{x_2} f^*(x) g_\alpha(x) g(x) dx \quad (A.2)$$

where

$$g_\alpha(x) = \frac{\gamma(x/\alpha)}{\int_{-\infty}^{\infty} \gamma(x/\alpha) dx} \quad (A.3)$$

$$\gamma(t) = \begin{cases} 0 & |t| \geq 1 \\ \exp\left(\frac{1}{t^2-1}\right) & |t| < 1 \end{cases} \quad (A1.4)$$

and $D(\hat{p})$ will be determine below taking into account that (2.5) must be finite. In the Fig. 1 graphics of the bell functions are shown for different values of α .

Through translations of the bell functions to an arbitrary point x_0 the bilinear form $\delta(x - x_0)$ is defined. Similarly we

can define the extended Dirac delta $\tilde{\delta}$ in the sense of (A.2), by semi-bell functions on the boundary points x_1 and x_2 (fig. 2) from which we obtain $\tilde{\delta} = \delta(x - x_2) - \delta(x - x_1)$.

At this point we ask what is the result of taking the limits $x_1 \rightarrow -\infty$ and $x_2 \rightarrow \infty$ in the relationship

$$\langle f | \hat{p} | g \rangle = \langle f | (-i\tilde{\delta} - \hat{p}^\dagger) | g \rangle \quad (2.13)$$

From Holder's inequality we have

$$\begin{aligned} \left| \int_{x_1}^{x_2} f^*(x) \hat{p}g(x) dx \right| &= \int_{x_1}^{x_2} |f^*(x) \hat{p}g(x)| dx \\ &\leq \int_{x_1}^{x_2} |f^*(x)|^2 dx \int_{x_1}^{x_2} |\hat{p}g(x)|^2 dx \end{aligned}$$

from where we conclude that limits $x_1 \rightarrow -\infty, x_2 \rightarrow \infty$, exist if $f \in L^2(R)$ and $\hat{p}g(x) \in L^2(R)$. Considering now

$$\int_{x_1}^{x_2} g(x) \hat{p}f^*(x) dx$$

we find that $g(x) \in L^2(R)$ and $\hat{p}f^*(x) \in L^2(R)$, from which it follows that f, g and their derivatives must belong to $L^2(R)$. Therefore $D(\hat{p}) = C^1(R) \cap L^2(R)$. From this and (2.13) we find that

$$\lim_{\substack{x_1 \rightarrow -\infty \\ x_2 \rightarrow \infty}} \tilde{\delta}(x, x_1, x_2)$$

must exists. In summary, we found two important facts:

- a) $f, g \in D(\hat{p})$.
- b) The limits $\lim_{x_1 \rightarrow -\infty} f(x_1)g(x_1)$ and $\lim_{x_2 \rightarrow \infty} f(x_2)g(x_2)$ exist.

From the condition a) the following limit

$$\langle f | \hat{p} | g \rangle + \langle g | \hat{p} | f \rangle^*$$

exists. From condition b) and (2.13) this limit is equal to

$$\lim_{\substack{x_1 \rightarrow -\infty \\ x_2 \rightarrow \infty}} [f(x_2)g(x_2) - f(x_1)g(x_1)]$$

The limits of the condition b) have to be zero, since otherwise $f y g$ will not satisfy condition a) because the integrals are not finite. Finally, we have that $\int c(\rho) d\rho = e$ because a primitive of the $\delta(x)$ is the Heaviside step function. For $\tilde{\delta}$ its primitive is given by $\tilde{H}(x) = H_{x_2}(x) - H_{x_1}(x)$ where

$$H_{x_k} = \begin{cases} 1 & \text{if } x \geq x_k \\ 0 & \text{if } x < x_k \end{cases}$$

for $k = 1, 2$.

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