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On Application of Unbounded Hilbert Linear Operators in Quantum Mechanics

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ABSTRACT

This research work presents an important Banach space in functional analysis which is known and called Hilbert space. We verified the crucial operations in this space and their applications in physics, particularly in quantum mechanics. The operations are restricted to the unbounded linear operators densely defined in Hilbert space which is the case of prime interest in physics, precisely in quantum machines. Precisely, we discuss the role of unbounded linear operators in quantum mechanics, particularly, in the study of Heisenberg uncertainty principle, time-independent Schrödinger equation, Harmonic oscillation, and finally, the application of Hamilton operator. To make these analyses fruitful, the knowledge of Hilbert spaces was first investigated followed by the spectral theory of unbounded operators, which are claimed to be densely defined in Hilbert space. Consequently, the theory of probability is also employed to study some systems since the operators used in studying these systems are only dense in H (i.e., they must (or probably) be in the domain of H defined by $L_2(-\infty,+\infty)$).

Key words: Normed and hilbert spaces, unbounded linear operators, unitary operators, spectral theory, schrödinger equation

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INTRODUCTION

Inner Product; Hilbert Space

Let X be a linear space. An inner product on X is a mapping $\langle,\rangle : X\times X \to \mathbb{C}$ defined on $X\times X$ with values in $\mathbb{C}$ (the set of complex numbers) such that the following conditions are satisfied for the vectors $x, y, z \in X$ and $\alpha, \beta \in \mathbb{C}$ scalars that is

$l_1 : \langle x, y\rangle \geq 0$ and $\langle x, y\rangle = 0 \Leftrightarrow x = y$

$l_2 : \langle x, y\rangle = \overline{\langle y, x\rangle}$ (the bar indicates complex conjugation)

$l_3 : \langle \alpha x + \beta y, z\rangle = \alpha\langle x, z\rangle + \beta\langle y, z\rangle$ where the pair $(X, \langle\cdot\rangle)$ is called an inner product space. Hilbert space is, therefore, a complete inner product space, where the completeness of this space can be verified in the metric defined by inner product on X as

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$$d(x,y)=\|x-y\|=\sqrt{\langle x-y,x-y\rangle}$$

and A norm on X is defined by $\|x\|=\sqrt{\langle x,x\rangle}$. Hence, inner product spaces are normed spaces while Hilbert spaces are Banach spaces.

Basic Properties

Here [Guisti, Enrico (1997)], we wish to establish some basic properties of a Hilbert space which shall be unavoidably recognized in this work. Observe first that an immediate consequence of l_2 and l_3 is that for arbitrary vectors $x,y,z\in X$ and $\alpha,\beta\in\mathbb{C}$, we have $\langle z,\alpha x+\beta y\rangle=\bar{\alpha}\langle z,x\rangle+\bar{\beta}\langle z,y\rangle$.

Therefore,

$$\langle z,\alpha x+\beta y\rangle=\overline{\langle \alpha x+\beta y,z\rangle}$$

by $l_2=\overline{\alpha\langle x,z\rangle+\beta\langle y,z\rangle}$, by $l_3=\bar{\alpha}\langle\overline{x,z}\rangle+\bar{\beta}\langle\overline{y,z}\rangle$ and by property of $\mathbb{C}=\bar{\alpha}\langle z,x\rangle+\bar{\beta}\langle z,y\rangle$ by l_2.

Cauchy Schwartz Inequality

Given X, a Hilbert space for arbitrary $x,y\in X$ we [Wittle, 1990] has

$$|\langle x,y\rangle|^2\le\langle x,y\rangle.\langle x,y\rangle\Rightarrow|\langle x,y\rangle|^2\le\|x\|\cdot\|y\|$$

Proof: Taking $x,y\in X$ to be arbitrary, let $z\in\mathbb{C}$ with $|z|=1$ and $z\langle x,y\rangle=|\langle x,y\rangle|$. Now, let $a=\langle x,x\rangle, b=|\langle x,y\rangle|$ and $c=\langle y,y\rangle$. Then, for arbitrary scalar $t\in\mathbb{R}$, we have

$$\begin{aligned}0&\le\langle tzx+y,tzx+y\rangle=t^2z\bar{z}\langle x,x\rangle+tz\langle x,y\rangle+t\bar{z}\langle x,y\rangle+\langle y,y\rangle\\&\le at^2+2t|\langle x,y\rangle|+c\Rightarrow at^2+2bt+c\end{aligned}$$

Solving quadratically, $b^2\le ac$, that is $|\langle x,y\rangle|^2\le\langle x,x\rangle\cdot\langle y,y\rangle$. Consequently, $|\langle x,y\rangle|\le\|x\|\cdot\|y\|$.

Norm on Hilbert Space

The function [Brenner, Scott (2005)] $\|\cdot\|:X\to\mathbb{R}$ defined by $\|x\|=\sqrt{\langle x,x\rangle}$ is a norm on X

Proof: That this norm holds follows from the definition of $\|\cdot\|$ and conditions l_1 and l_2. Since for a linear space X over K to be called a normed linear space defined as a real-valued function $\|\cdot\|$ by $\|\cdot\|:X\to[0,\infty]$, the followings are satisfied.

$N_1:\|x\|\ge 0$ and $\|x\|=0\Leftrightarrow x=0$

$N_2:\|kx\|=|k|\|x\|$ for all $k\in K, x\in X$

$N_3:\|x+y\|\le\|x\|+\|y\| \quad \forall x,y\in X$

It now suffices to verify N_3. For arbitrary $x, y, z \in X$

$$\begin{aligned}\|x+y\|^2 &= \langle x+y, x+y\rangle = \langle x, x+y\rangle + \langle y, x+y\rangle \\ &= \langle x,x\rangle + \langle x,y\rangle + \langle y,x\rangle + \langle y,y\rangle = \|x\|^2 + \left(\langle x,y\rangle + \overline{\langle x,y\rangle}\right) + \|y\|^2 \\ &= \|x\|^2 + 2\operatorname{Re}\langle x,y\rangle + \|y\|^2 \le \|x\|^2 + 2\left|\langle x,y\rangle\right| + \|y\|^2 \\ &= \|x\|^2 + 2\|x\|\cdot\|y\| + \|y\|^2 = \left(\|x\| + \|y\|\right)^2\end{aligned}$$

Hence, the result follows.

1.1. The parallelogram Law

Let X be an inner product space [Dunford, Schwatz (1998)], then arbitrary $x, y \in X$ we have $\|x+y\|^2 + \|x-y\|^2 = 2\left(\|x\| + \|y\|\right)^2$. As in the case of the latter proof, by expanding the LHS, the RHS will be obtained immediately.

Orthogonality of Inner Product Spaces

Here [Halmes, 1992], two vectors x and y in an inner product space X are said to be orthogonal usually denoted by $x \perp y$ or $y \perp x$, if and only if $\langle x, y\rangle = 0$.

This very property will play important roles in this work. The exhibition of Hilbert space properties has to stop here and every other relevant ones shall be explained alongside their applications.

Linear Operators in Hilbert Spaces

We continue in this section by considering linear operators $T : D(T) \to H$ whose domain $D(T)$ lies in a complex Hilbert space H. Here, we admit that such an operator T may be UNBOUNDED, that is, may not be bounded. For a bounded operator, we say that a linear operator is bounded if and only if there is a real number $c \ni \forall x \in D(T), \|Tx\| \le c\|x\|$. But here [Baurbaki, 1997], we expect an unbounded linear operator to be different from a bounded one in various ways, hence, these results in many questions on what properties we should focus our attention on. A famous result shall be obtained from the theorem of boundedness given below. We shall see that the result suggests that the domain of the operator and the problem of extending the operator will play a remarkable role.

Boundedness

Theorem 1.7.1 [Hellinger-Toe Plitz theorem]: A linear operator T [Courand and Hilbert (1993)] defined on all of a complex Hilbert space H which satisfies the relation, for all $x, y \in H$ a bounded linear operator

$$\langle Tx, y\rangle = \langle x, Ty\rangle \tag{1}$$

Proof: Suppose H would contain a sequence (y_n) such that $\|y_n\| = 1$ and $\|Ty_n\| \to \infty$, we consider the functional f_n defined by $f_n(x) = \langle Tx, y_n\rangle$ where $n = 1, 2, \ldots$ and we use (1). Each f_n is defined in all of H and is linear. For each fixed n the functional f_n is bounded since the Schwartz inequality gives

$$|f_n(x)| = |\langle x, Ty_n\rangle| \le \|Ty_n\|\|x\|$$

From this and the knowledge of uniform boundedness which can be easily verified from the above prove, we conclude that $\left(\|f_n\|\right)$ is bounded say, $\|f_n\| \le k \forall n$. This implies that for every $x \in H$, we have

$$|f_n x| \le \|f_n\|\|x\| \le k\|x\|$$

And taking $x = Ty_n$, we have

$$\|Ty_n\|^2 = \langle Ty_n, Ty_n \rangle = |f_n(Ty_n)| \le k\|y_n\|$$

Hence $\|Ty_n\| \le k$ and the initial assumption is contradicted for $\|Ty_n\| \to \infty$ hence completing the proof.

Domains and extensions

Since by the theorem above, $D(T) = H$ is not possible for unbounded linear operators satisfying (1), we are, therefore, confronted with the problem of determining suitable domains and extensions problem. Consider [Hewitt and Stromberg (1995)] the relation: $S \subset T$

This relation simply means that the operator T is just an extension of another operator S, thus $D(S) \subset D(T)$ and $S = T|_{p(s)}$ where the extension T of S is called a proper extension in the sense that for $D(S)$ being a subset of $D(T)$, $D(T) - D(S) \ne 0$. In the theory of bounded operators, the Hilbert adjoint operator denoted by T^* of an operator T plays a basic role. Therefore, to make this section fruitful, we shall generalized this important concept to unbounded operators. In the case of bounded operator T^* defined by

$$\langle Tx, y \rangle = \langle x, y^* \rangle \tag{2}$$

which can be written as

(a) $\langle Tx, y \rangle = \langle x, y^* \rangle$

(b) $y^* = Ty^*$

where T^* is bounded with norm $\|T^*\| = \|T\|$.

Now in the case of which unbounded operator T^* for each $y \in D(T^*)$ the corresponding $y^* = T^* y$ must be unique. Here, we claim that it is true if and only if T is DENSLY define in H (i.e., $D(T)$ is dense in H)

Further, if $D(T)$ is not dense in H, then $\overline{D(T)} \ne H$. The orthogonal complement of $\overline{D(T)}$ in H contains a nonzero y_1 and $y^{\perp} x \forall x \in D(T)$. That's $\langle x, y_1 \rangle = 0$. But then in Equation (2), we obtain

$$\langle x, y^* \rangle = \langle x, y^* \rangle + \langle x, y_1 \rangle = \langle xy^* + y_1 \rangle$$

which shows non-uniqueness. On the other hand, if $D(T)$ is dense in H, then $D(T)^{\perp} = \{0\}$. Hence, $\langle x, y_1 \rangle = 0 \quad \forall x \in D(T)$.

Now, this implies that $y_1 = 0$ so that $y^* + y_1 = y^*$ which entails uniqueness.

Unbounded Hilbert adjoint operator

Definition [**Arkangel, Skic (2001)]**: Let $T : D(T) \to H$ be a (possibly unbounded) densely defined linear operator in a complex Hilbert space H. Then, the Hilbert adjoint operator.

$T^* : D(T^*) \to H$ of T is defined as the domain $D(T^*)$ of T^* which consist of all $y \in H$ $\exists y^* \in H$ satisfying

$$\langle Tx, y\rangle = \langle x, y^*\rangle \quad \forall x \in D(T) \tag{3}$$

The Hilbert adjoint operator T^* is then defined in term of y^* by $y^* = T^* y \quad \forall y \in H$ is also in $D(T^*)$.

Theorem 2 (**Hilbert adjoint operator**):[1] Let $S : D(S) \to H$ and $T : D(T) \to H$ be linear operators densely defined in a complex Hilbert space H, then,

a. If $S \subset T$, then $T^* \subset S^*$

b. If $D(T^*)$ is dense in H, then $T \subset T^{**}$

Proof:

(a) By the definition of T^* we have $\langle Tx, y\rangle = \langle x, T^* y\rangle$ $\forall x \in D(T)$ and $\forall y \in D(T^*)$

Recall that $S \subset T$, this implies that $\langle Sx, y\rangle = \langle x, T^* y\rangle$ $\forall x \in D(s)$ and y as before then by definition of S^*, $\langle Sx, y\rangle = \langle x, S^* y\rangle$, $\forall x \in D(s)$ and $\forall y \in D(S^*)$, our target is to show that $D(T^*) \subset D(S^*)$.

Recall by the definition of Hilbert adjoint operator S^*, the domain $D(S^*)$ includes all y for which one has a representation (3) of $\langle Sx, y\rangle$ with x varying throughout $D(S)$ and also in Equation (2) then, the set of $y's$ for which Equation (2) is valid must be (either proper or improper) subset of $y's$ for which Equation (3) holds. That is, we must have $D(T^*) \subset D(S^*)$ so, from Equations (2) and (3) we conclude that $S^* y = T^* y$ $\forall y \in D(T)$. Hence, $T^* \subset S^*$ by definition.

(b) Taking complex conjugates in Equation (1), we have, $\langle T^* y, x\rangle = \langle y, Tx\rangle$ $\forall y \in D(T^*)$ and $x \in D(T^{**})$. Since $D(T^*)$ is dense in H, the operator T^{**} exists and by the definition $\langle T^* y, x\rangle = \langle y, Tx\rangle \forall y \in D(T^*)$, $x \in D(T^{**})$ as in Equation (4) and this very definition, reasoning as in part (a) we conclude that $x \in D(T)$ also belongs to $D(T^{**})$. Hence, $T^{**}x = Tx \Leftrightarrow T \subset T^{**}$. Note that $(T^*)^* = T^* = T$ for bounded linear operators.

Symmetric linear operator

Definition: Let $T : D(T) \to H$ be a linear operator, which is unbounded but densely defined in a complex Hilbert space H. Then, T is called a symmetric linear operator if for all we have, $\langle Tx, y\rangle = \langle x, Ty\rangle$. Here, it is quite remarkable that symmetry can be expressed in terms of Hilbert adjoint operators in a simple fashion. So, we shall use this expression in further work.[2]

Lemma1.7.4 (SYMMETRIC OPERATOR): A densely defined liner operator T in a complex Hilbert space H is Symmetric if and only if $T \subset T^*$

Proof: The definition relation of T^*, $\langle Tx, y\rangle = \langle x, T^* y\rangle$ is valid for all $x \in D(T)$ and $y \in D(T^*)$. Assuming that $T \subset T^*$, we have $T^* y = Ty$ $\forall x, y \in D(T)$ so that (1) for $x, y \in D(T)$ becomes $\langle Tx, y\rangle = \langle x, Ty\rangle$. Hence, T is symmetric.

Self Adjoint linear operator

Definition: Let the mapping $T : D(T) \to H$ be a linear operator, which is densely defined in a complex Hilbert space H. Then, T is called a self adjoint linear operator if and only if $T = T^*$.[3]

By virtue of this, every self-adjoint linear operator is symmetric. On the other hand, a symmetric linear operator need not be self-adjoint. This is because T^* may be a proper extension of T, that is $D(T) \neq D(T^*)$. It is obvious that this cannot be possible if $D(T)$ is all of H, so we have that for a linear operator $T : H \to H$ on a complex Hilbert adjointness are identical. In this case, T becomes bounded. Hence, we concluded that a densely defined linear operator T in complex Hilbert space H is symmetric if and only if $\langle Tx, x\rangle$ is real for all $x \in D(T)$.

Closed linear operators

Definition: Let $T : D(T) \to H$ be a linear operator, where $D(T) \subset H$ and is a complex Hilbert space. Then, T is called a closed linear operator if its graph[4]

$$\vartheta(T) = \{(x, y) | x \in D(T), y = Tx\}$$

is closed in $H \times H$ where the norm on $H \times H$ is defined by

$$\|(x, y)\| = \left(\|x\|^2 + \|y\|^2\right)^{1/2}$$

Theorem 1.7.6: Let $T : D(T) \to H$ be a linear operator where $D(T) \subset H$ and is a complex Hilbert space then:

(a) T is closed if and only if $x_n \to x, [x_n \in D(T)]$ and $Tx_n \to y$ together imply that $x \in D(T)$ and $Tx = y$

(b) If T is closed and $D(T)$ is closed, then T is bounded

SPECTRAL THEORY OF UNBOUNDED LINEAR OPERATORS

For unbounded linear operator, the same general properties of the spectrum that holds in bounded operators also hold in the unbounded operators particularly in the case of self-adjoint linear operators. Here, the whole spectrum as in the bounded cases continues to be real and closed although it will no longer be bounded. To show this reality, we consider the generalized theorem as follows which proof follows the method used in the case of bounded operators.

Theorem 2.1 (Regular values):[5] Let $T : D(T) \to H$ be a self-adjoint linear operator which is densely defined in a complex Hilbert space H. Then, a number λ belongs to the resoluent set $\rho(T)$ of T if and only if there exists a $C > 0$ such that for every $x \in D(T)$, $\|T_\lambda x\| \geq C\|x\|$ where $T_\lambda = T - \lambda I$.

Proof:

(a) Let $\lambda \in \rho(T)$ then be the following definition, let $X \neq \{0\}$ be a complex normed space and $T : D(T) \to X$ a linear operator with domain $D(T) \subset X$. A regular value λ of T is a complex number such that:

$(R_1): R_\lambda(T)$ exists,

$(R_2): R_\lambda(T)$ is bounded

$(R_3): R_\lambda(T)$ is defined on a set which is dense in X

Then, $R_\lambda = (T-\lambda)^{-1}$ exists and is bounded say $\|R_\lambda = k > 0\|$. Consequently, since $R_\lambda T_\lambda x = x$ for $x \in D(T)$ we have

$$\|x\| = \|R_\lambda T_\lambda x\| \le \|R_\lambda\|\|T_\lambda x\| = k\|T_\lambda x\|$$

Dividing by K, we have $\|T_\lambda x\| \ge C\|x\|$ where $C = 1/K$.

Conversely, suppose that (1) holds for some $c > 0$ and all $x \in D(T)$. We consider the vector space $Y = \{y / y = T_\lambda x, x \in D(T)\}$, that is, the range of T_λ and show that

i. $T_\lambda : D(T) \to Y$ is bijective

ii. Y is dense in H

iii. Y is closed

Together, this implies that the resolvent $R_\lambda = T_\lambda^{-1}$ is defined on all of H. Boundedness of R_λ will then easily result from Equation (1) so that $\lambda \in \rho(T)$. The details are as follows;

Consider any $x_1, x_2 \in D(T)$ such that $T_\lambda x_1 = T_\lambda x_2$. Since T_λ is linear, then Equation (1) holds

$$0 = \|T_\lambda x_1 - T_\lambda x_2\| = \|T_\lambda (x_1 - x_2)\| \ge c\|x_1 - x_2\|$$

but $c > 0$ implies that $\|x_1 - x_2\| = 0$. Hence, $x_1 = x_2$, so that the operator $T_\lambda : D(T) \to Y$ is bijective. We now prove that $\bar{Y} = H$ by showing that $x_0 \perp Y$ then for every $y = T_\lambda c \in Y$

$$0 = \langle T_\lambda x, x_0 \rangle = \langle Tx, x_0 \rangle - \lambda \langle x, x_0 \rangle$$

Hence, for all $x \in D(T), \langle Tx, x_0 \rangle = \langle x, \bar{\lambda} x_0 \rangle$ by definition of Hilbert adjoint operator, this shows that $x_0 \in D(T^*)$ and $T^* x_0 = \bar{\lambda} x_0$. Since T is self-adjoint operator, this shoes that $x_0 \in D(T^*)$ and $T^* x_0 = \bar{\lambda} x_0$. Since T is self-adjoint, $D(T^*) = D(T)$, and $T^* = T$: thus $Tx_0 = \bar{\lambda} x_0$ where $x_0 \ne 0$ would imply that $\bar{\lambda}$ is eigenvalue of T and then $\bar{\lambda} = \lambda$ must be real hence, $Tx_0 = \lambda x_0$, that is, $T_\lambda x_0 = 0$ but the Equation (1) yields a contradiction:

$$0 = \|T_\lambda x_0\| \ge c\|x_0\| \Rightarrow \|x_0\| = 0$$

It follows that $\bar{Y}^\perp = \{0\}$, so $\bar{Y} = H$ (by theorem of direct sum).

Now, we want to prove that Y is closed. Let $y_0 \in \bar{Y}$ then there is a sequence $\{y_n\}$ in Y such that $y_n \to y_0$. Since $y_n \in Y$, we have $y_n = T_\lambda x_n$ for some $x_n \in D(T_\lambda) = D(T)$ then by Equation (1) above

$$\|x_n - x_m\| \le 1/c \|T_\lambda (x_n - x_m)\| = 1/c \|y_n - y_m\|$$

But y_n is convergent, so x_n is closed. Also since H is complete, $\{x_n\}$ converges say $x_n \to x_0$. In addition, since T is self-adjoint, it is closed because the Hilbert adjoint operator T^* is closed. Theorem 1.7.6 thus implies that we have $x_0 \in D(T)$ and $T_\lambda x_0 = y_0$ this implies that $y_0 \in \bar{Y}$. Since $y_0 \in \bar{Y}$ was arbitrary, Y is closed. Hence, part (ii) and (iii) imply that $Y = H$ and (i) we see that the resolvent R_λ exists and if defined on all of H:

$$R_\lambda = T_\lambda^{-1}; H \to D(T)$$

Here, the boundedness of R_λ is from Equation (1) above because $\forall y \in H$ and corresponding $x = R_\lambda y$, we have $y = T_\lambda x$ and by Equation (1) $\|R_\lambda y\| = \|x\| \le \frac{1}{c}\|T_\lambda x\| = \frac{1}{c}\|y\|$ so that $\|R_\lambda\| \le {}^{1}\!/_{C}$ and by definition, this proves that $\lambda \in \rho(T)$. Now, we wish to show that in the case of unbounded self-adjoint linear operators that its spectrum is real.

Theorem 2.2 (Spectrum): The spectrum $\sigma(T)$ of a self-adjoint linear operator $T : D(T) \to H$ is real and closed. Here, H is a complex Hilbert space and $D(T)$ is dense in H.

Proof (The reality of $\sigma(T)$): For every $x \ne 0$ in $D(T)$ we have $\langle T_\lambda x, x\rangle = \langle Tx, x\rangle - \lambda\langle x, x\rangle$ and since $\langle x, x\rangle$ and $\langle T_\lambda, x\rangle$ are real then $\langle T_\lambda x, x\rangle = \langle Tx, x\rangle - \bar{\lambda}\langle x, x\rangle$ where $\lambda = \alpha + i\beta$ with real α and β. Then, $\bar{\lambda} = \alpha + i\beta$ so by subtraction

$$\overline{\langle T_\lambda x.x\rangle} - \langle T_\lambda x, x\rangle = (\lambda - \bar{\lambda})\langle x, x\rangle = 2i\beta\|x\|^2$$

The left side equals $-2ilm\langle T_\lambda x, x\rangle$. Since the imaginary part of a complex number cannot exceed the absolute value, we have by Schwartz inequality

$$|\beta|\|x\|^2 \le |\langle T_\lambda x, x\rangle| \le \|T_\lambda x\|\|x\|$$

Dividing by $\|x\| \ne 0$ we have $|\beta|\|x\| \le \|T_\lambda x\|$ $\forall x \in D(T)$ but if λ is not real, $\beta \ne 0$ so that $\lambda \in \rho(T)$ by the previous theorem. Hence, $\sigma(T)$ must be real.

Proving the closeness of (T). Here, we wish to prove that $\sigma(T)$ is closed if we can succeed in showing that the resolvent set $\rho(T)$ is open. Now, let $\lambda_0 \in \rho(T)$, it is to show that for every λ sufficiently close to λ_0 also belongs to $\rho(T)$. By the triangle inequality, we have

$$\|T_\lambda - \lambda_0 x\| = \|Tx - \lambda x + (\lambda - \lambda_0)x\| \le \|Tx - \lambda x\| + |\lambda - \lambda_0|\|x\|$$

We can also see it this way

$$\|Tx - \lambda x\| \ge \|Tx - \lambda_0 x\| - |\lambda - \lambda_0\|x\||$$

Since $\lambda_0 \in \rho(T)$ by theorem (2.2) there exist a constant $c > 0 \ni \forall x \in D(T)$, $\|Tx - \lambda_0 x\| \ge c\|x\|$

We can assume that λ is close to λ_0 say $\|\lambda - \lambda_0\| \leq \frac{c}{2}$ then Equations (2) and (3) imply that $\forall x \in D(T)$

$$\|Tx - \lambda_0 x\| \geq c\|x\| - \frac{1}{2}c\|x\| = \frac{1}{2}c\|x\|$$

Hence, $\lambda \in \rho(T)$ by theorem (2.1). Since λ was such that $|Tx - \lambda_0 x| \leq \frac{c}{2}$ though arbitrary, this shows that λ_0 has a neighborhood belonging to entire $\rho(T)$. Since λ_0 was arbitrary, we conclude that $\rho(T)$ is open hence $\sigma(T) = C - \rho(T)$ is closed.

Spectral Representation of Unitary Operator

Our main goal here is to establish a spectral representation of self-adjoint linear operators that may be unbounded. This can be achieved from the spectral presentation of unitary operators. To do this, we investigate the spectral theorem for unitary operators first.

Theorem 2.1. (Spectrum): If $U : H \to H$ is a unitary linear operator on a complex Hilbert space $H = \{0\}$, then the spectrum $\sigma(u)$ is a closed subset of the unit circle; thus $|\lambda| = 1, \forall \lambda \in \sigma(u)$.

Proof: By the theorem of unitary operator, $\|U\| = 1$, hence $|\lambda| \leq 1\ \forall \lambda \in \sigma(U)$ also $0 \in \rho(u)$ since for $\lambda = 0$ the resolvent operator of U becomes $U^{-1} = U^*$. The operator U^{-1} is unitary, hence $\|U^{-1}\| = 1$.

Let $T = U$ and $\lambda_0 = 0$, this now implies that every λ satisfying $|\lambda| < 1/\|U^{-1}\| = 1$ belongs to $\rho(U)$ (form resolvent spectrum theorem). Hence, the spectrum of U must lie on the unit circle. Therefore, it is closed by the closed spectrum theorem which say that if the resolvent set $\rho(T)$ is open, its spectrum $\sigma(T)$ is closed.

Wecken's Lemma (2.1.1):[6] Let w and A be bounded self-adjoint linear operators on a complex Hilbert Space H. Suppose that $WA = AW$ and $W^2 = A^2$. Let P be the projection of H onto the null space $N(W - A)$, then:

(a) If a bounded linear operator commutes with $W - A$ it also commute with P

(b) $Wx = 0$ implies $Px = x$

(c) We have $W = (2p - 1)A$

Proof:

a. Suppose that B commutes with $W - A$ since we have $Px \in N(W - A)\ \forall x \in H$

We obtain: $(W - A)BPx = B(w - A)P(x) = 0$. This shows that $BPx \in N(W - A)$ and this implies $P(BP_x) = BP_x$ that is

$$PBP = BP \cdots \quad (4)$$

Showing this relation, since $W - A$ is self-adjoint we have

$$(W - A)B^* = \left[B(W - A)\right]^* = \left[(W - A)B^*\right] = B^*(W - A)$$

This shows that B^* and $(W - A)$ commute. So with the reasoning from above, we $PB^*P = B^*P$ as the analogue of Equation (4). Since projections are usually self-adjoint, it follows that $PBP = \left(PB^*P\right)^* = PB$

therefore, together with Equation (4) we have $BP = PB$.

(b). Let $Wx = 0$, since A and W are self-adjoint, moreover, $A^2 = W^2$ we obtain

$$\|A_x\|^2 = \langle Ax, Ax\rangle = \langle A^2x, x\rangle = \langle W^2x, x\rangle = \|Wx\|^2 = 0$$

That is $Ax = 0$. Hence, $\langle W - A\rangle x = 0$. This shows that $x \in N(W - A)$. Consequently, $Px = x$ since p is the projection of H onto $N(W - A)$.

(c). From the assumption $W^2 = A^2$ and $WA = AW$, we have

$$(w - A)(w + A) = w^2 - A^2 = 0$$

Hence, $(w + A)x \in N(w - A)x \quad \forall x \in H$. Since P projects H onto $N(W - A)$, we thus obtain $P(W + A)x = (W + A)x, \forall x \in H$ that is $P(W + A) = W + A$.

Now, $P(W - A) = (W - A)P$ by (a) and $(W - A)P = 0$. Since P projects H onto $N(W - A)$. Then, $2PA = P(W + A) - P(W - A) = W + A$, we see that $2PA - A = W$ which proves (c). The desired spectral theorem can now be formulated as follows.

THEOREM (2.1.2) (SPECTRAL THEOREM FOR UNITARY OPERATORS)[7]

Let $U : H \to H$ be a unitary operator on a complex Hilbert space $H \neq \{0\}$ then

$$U = \int_{-\pi}^{\pi} e^{i\theta} dE_\theta = \int_{-\pi}^{\pi} (\cos\theta + i\sin\theta) dE_\theta \tag{5}$$

There exists spectral family $\varepsilon = (E_\theta)$ on $[-\neq, \neq]$ such that

$$U = \int_{-\pi}^{\pi} e^{i\theta} d\varepsilon = \int_{-\pi}^{\pi} (\cos\theta + i\sin\theta) d\varepsilon \tag{6}$$

More generally, for every continuous function f defined on the unit circle

$$f(U) = \int_{-\pi}^{\pi} f(e^{i\theta}) dE_\theta$$

Then for $x, y \in H$,

$$\langle f(U)x, y\rangle = \int_{-\pi}^{\pi} f(e^{i\theta}) dw(\theta), w(\theta) = \langle E_\theta\, x, y\rangle \tag{6*}$$

Where the integral an ordinary Riemann integral.

Proof:

Here, we want to prove that for a given unitary operator U there is a bounded self-adjoint operator S with

$$\sigma(S) \subset [-\pi, \pi] \ni U = e^{is} = \cos S + i\sin S \tag{7}$$

Here, we wish to prove step wisely that

a. U in (7) is unitary provided that S exists

b. Let $U = V + iW$ where $V = \frac{1}{2}(U + U^*)$ and $W = \frac{1}{2i}(U - U^*)$ that V and W are self-adjoint and there exists $-1 \le V \le 1$ and $-1 \le W \le 1$

c. We shall investigate some properties of $g(V)$ for $g(V)=\arccos V$ and $A=\sin g(V)$

d. Then finally, we shall prove that the desired operator S given by

$$S=(2p-1)(\arccos V)$$

where P is the projection of H onto $N(W-A)$. So may we start this way;

(a) If S is bounded and self-adjoint so are $\cos S$ and $\sin S$ by the following lemma.

Power series
Lemma 2.1.2 (Power Series)
Let

$$h(\lambda)=\sum_{n=0}^{\infty}\alpha_n\lambda^n;(\alpha_n \text{ real})$$

Be absolutely convergent for all λ such that $|\lambda|\le k$. Suppose that $S\in B(H,H)$ is self-adjoint and has norm $\|S\|\le k, H$ is a complex Hilbert space then $h(S)=\sum_{n=0}^{\infty}|\alpha_n|S^n$ is a bounded self-adjoint linear operator and $\|h(S)\|\le\sum_{n=0}^{\infty}|\alpha_n|k^n$.

If a bounded linear operator commutes with S, it also commutes with $h(S)$. Hence, these operators above commute likewise. This, therefore, implies that U in Equation (7) is unitary since, by the theorem of unitary operator, we have

$$UU^*=(\cos S+i\sin S)(\cos S-i\sin S)=(\cos S)^2+(\sin S)^2$$
$$=(\cos^2+\sin^2)(S)=1 \text{ and similarly, } U^*U=1$$

From the proof of (a), we observed that $UU^*=U^*U=1$, therefore, we have from Equation (9)

$$VW=WV \qquad (12)$$

Also, $\|U\|=\|U^*\|$ this implies

$$\|U\|=\|U^*\|=1 \text{ and } \|V\|\le\|W\|\le 1 \qquad (13)$$

Hence, the Schwartz inequality yields $|\langle Vx,x\rangle|\le\|Vx\|\|x\|\le\|V\|\|x\|^2\le\langle x,x\rangle$.

That is $-\langle x,x\rangle\le\langle Vx,x\rangle\le\langle x,x\rangle$ this proves the formula (10) above; $-1\le V\le 1\equiv -1\le W\le 1$ then, the second one follows by the same argument.
Furthermore, from Equation (9), we obtain

$$V^2+W^2=1 \qquad (14)$$

$$g(\lambda)=\arccos\lambda=\pi/2-\arcsin\lambda=\frac{\pi}{2}-\lambda-\frac{1}{6}\lambda^3+\frac{1}{120}\lambda^5-\cdots$$

This Maclaurin series on the right converges for $|\lambda|\le 1$. It is wise knowing that the convergence at $\lambda=1$ follows by knowing that the series of $\arcsin\lambda$ as established above has positive coefficients.

Hence, a monotone sequence of partial sums S_n when $\lambda>0$, which is bounded on $(0,1)$ since

$S_n(\lambda) < \arcsin\lambda < \pi/2$, so that for every fixed n we have $S_n(1) \leq \pi/2$ as $\lambda \to 1$.

Convergence at $\lambda = -1$ follows readily from that at $\lambda = 1$

Now by Equation (13), $\|\lambda\| \leq 1$, then, the lemma (2.1.2) (power series) implies here that the operator

$$g(v) = \arccos V = \frac{\pi}{2} - V - 1/6\,V^3 + \cdots \tag{15}$$

exists and is self-adjoint. We now define

$$A = \sin g(V) \tag{16}$$

This is a power series in V, therefore, the lemma (2.1.2) implies that A is a self-adjoint and commutes with V and by Equation (12), also with W since by Equation (15) we establish

$$\cos g(v) = V \tag{17}$$

We have $V^2 + A^2 = (\cos^2 + \sin^2)(g(v)) = I$. Comparing this result with Equation (14), we have $W^2 = A^2$. Hence, we can apply Wecken's lemma and conclude that

$$W = (2p-1)A \tag{18}$$

Then that $Wa = 0$ implies $Px = x$ and P commutes with V and with $g(V)$ since these operators commute with $W - A$

$$S = (2p-1)g(V) = g(V)(2p-1) \tag{19}$$

We now define obviously, S is self-adjoint. We can now prove that S satisfies Equation (7). So llet $k = \lambda^2$ and define h_1 and h_2 by;

$$\begin{aligned} h_1(k) &= \cos\lambda = 1 - \frac{1}{2!}\lambda^2 + \cdots \\ h_2(k) &= \sin\lambda = \lambda - \frac{1}{3!}\lambda^3 + \cdots \end{aligned} \tag{20}$$

These functions exist for all k. Since P is a projection, we have $(2p-1)^2 = 4p^2 - 4p + 1$, so that Equation (19) gives $S^2 = (2p-1)^2 g(v)^2 = g(v)^2$.

Hence, by Equation (17)

$$\cos S = h_1(S^2) = h_1\left(g(V)^2\right) = \cos g(v) = V$$

We show that $\sin S = W$

Using (20), (16) and (18), we have

$$\begin{aligned} \sin S &= Sh_2(S^2) = (2p-1)g(v)h_2\left(g(v)^2\right) \\ &= (2p-1)\sin g(v) = (2p-1)A = W \end{aligned}$$

Finally, we show that $\sigma(S) \subset [-\pi, \pi]$. Since $|\arccos \lambda| \leq \pi$, we conclude that $\|S\| \leq \pi$ since S is self-adjoint and bounded, $\sigma(S)$ is real.

Let (E_θ) be a spectral family of S then Equations (5) and (6) follow from Equation (7), for bounded self-adjoint operator. In summary, we could equally define E_θ by

$$E_\theta = \begin{cases} 0, & \text{if } \theta = -\pi \\ \bar{E}_\theta - \tilde{E}_{-\pi}, & \text{if } -\pi < \theta < \pi \\ 1 & \text{if } \theta = \pi \end{cases}$$

E_θ is continuous at $\theta = -\pi$, so that the lower limit of integration $-\neq$ in Equations (5) and (6) is in order.

Spectral representation of unbounded self-adjoint linear operators

We have been representing self-adjoint linear operators in bounded form using unitary operators. Now, we wish to derive a spectral representation for an unbound self-adjoint linear operator $T : D(T) \to H$ on a complex Hilbert space H, where $D(T)$ is considerably dense in H. For this purpose, we associate with T the operator

$$U = (T - i1)(T + i1)^{-1} \tag{1}$$

Where U is called the Casyley's transform of T. It is a unitary operator. Using U as a unitary operator, we shall prove the lemma (2.2.1) below and the reason for the approach is that we shall be able to obtain the spectral theorem for the unbounded T from that for the bounded operator U as shown above.

T has its spectrum $\sigma(T)$ on the real axis of the complex plane C, whereas the spectrum of a unitary operator lies on the unit circle of C. A mapping $C \to C$ which transforms the real axis into the unit circle is given by $U = \dfrac{t-i}{t+i}$, this suggests the Equation (1). Now, to prove U as a unitary operator we have this lemma.

Lemma (2.2.1a) (Cayley's Transform)[8]

The Cayley transform $U = (T - i1)(T + i1)^{-1}$ of a self-adjoint linear operator $T : D(T) \to H$ exists on H and is a unitary operator. Here, $H \neq \{0\}$ is a complete Hilbert space.

Proof:

Since T is self-adjoint, $\sigma(T)$ is real. Hence, i and $-i$ belong to the resolvent set $\rho(T)$ consequently by the definition of $\rho(T)$. The inverses $(T + i1)^{-1}$ and $(T - i1)^{-1}$ exist on a dense subset of H and are bunded operators. Now taking T as a closed operator, $T = T^*$ and those inverse are defined on also of H. That is,

$$R(T + i1) = H, R(T - i1) = H \tag{3}$$

We thus have that, since I is defined on all of H, then

$$(T + i1)^{-1}(H) = D(T + i1) = D(T) = D(T - i1)$$

As well as $(T - i1)(D(T)) = H$. This relationship shows that U in Equation (1) is a bijection of H onto itself. However, we are to prove that U is isometric. For this purpose, we take any $x \in H$, setting $y = (T + i1)^{-1} x$ and use $\langle y, Ty \rangle = \langle Ty, y \rangle$.

Then, we obtain the desired result by straightforward calculation

$$\|Ux\|^2 = \|(T - i1)y\|^2 = \langle Ty - iy, Ty - iy \rangle = \langle Ty, Ty \rangle + i\langle Ty, y \rangle - i\langle y, Ty \rangle + \langle iy, iy \rangle$$
$$= \langle Ty + iy, Ty + iy \rangle = \|(T + i1)y\|^2 = \left\|(T + i1)(T + i1)^{-1} x\right\|^2 \|Ux\|^2 = \|x\|^2$$

The result really convinces us that U is unitary since the Cayley transform U of T is unitary, U has a spectral representation for T. Hence, we are to obtain the spectral representation of T using U. For this reason, we express T in terms of U.

Lemma (2.2.1b) (Cayley Transform) [8]

Let T be as in the lemma above, and let U be defined by Equation (1) then:

$$T = i(1 + U)(1 - U)^{-1} \tag{4}$$

Let $x \in D(T)$ and

$$y = (T + i1)x \tag{5}$$

Then, $U_y = (T - i1)x$ because $(T + i1)^{-1}(T + i1) = 1$ by addition and subtraction, we obtain

a. $(1 - U)x = 2iy$

b. $(1 - U)y = 2ix$

From Equation (5) and we see that $y \in R(T + i1) = H$ and (6b) now shows that $1 - U$ maps H onto $D(T)$ and if $(1 - U)y = 0$, then $x = 0$, so that $y = 0$ by Equation (5).

Hence $(1 - u)^{-1}$ exists and is defined on the range of $I - U$ which is $D(T)$ by $(6b)$, then Equation (6) gives

$$y = 2i(1 - U)^{-1} x, (x \in D(T)) \tag{7}$$

By substitution into Equation (6a), we have

$$Tx = \tfrac{1}{2}(1 + U)y; Tx = i(1 + U)(1 - U)^{-1} x; Tx = i(1 + U)(1 - U)^{-1}$$

For all $x \in D(T)$, completing the proof of Equation (4). Conclusively, the result obtained by Equation (4) represents T as a function of the unitary operator U. Now, applying the spectral theorem of unitary operator (above), we set up the following theorem.

Theorem 2.2.3 (Spectral theorem for self-adjoint linear operators)[9]

Let $T : D(T) \rightarrow H$ be a self-adjoint linear operator, where $H \neq \{0\}$ is a complex Hilbert space and $D(T)$ is dense in H. Let U be the Cayley transform (as in Equation (1)) of T and (E_θ) the spectral family in the spectral representation of Equation (5) of $-U$, then for all $x \in D(T)$

$$\langle Tx,x\rangle = \int_{-\pi}^{\pi} \tan\frac{\theta}{2} dw(\theta), w(\theta) = \langle E_\theta x,x\rangle$$
$$= \int_{-\infty}^{\infty} \lambda dv(\lambda), v(\lambda) = \langle F_\lambda x,x\rangle \tag{8}$$

From the spectral theorem of unitary operator (2.1.2), we have

$$-U = \int_{-\pi}^{\pi} e^{i\theta} dE_\theta = \int_{-\pi}^{\pi} (\cos\theta + i\sin\theta) dE_\theta \tag{9}$$

While proving part (a), we showed that E_θ is continuous at $-\neq$ and $\neq$. This property is also needed in part (b) to establish Equation (8) above

Recall that (E_θ) is the spectral family of a bounded self-adjoint linear operator, so we denote it with S where, we have $-U = \cos S + i\sin S$. Here, it is obvious that the value θ_0 at which (E_θ) is discontinuous is called the eigenvalue of S. Hence, we take $x \neq 0 \ni Sx = \theta_0 x$ hence for any polynomial $q, \exists q(S)x = q(\theta_0)x$ for any continuous for g on $[-\pi,\pi]$

$$g(S)x = g(\theta_0)x \tag{11}$$

Since $\sigma(s) \subset [-\pi,\pi], E_{-\pi-0} = 0$. Hence, if $E_{-\pi} \neq 0$ it implies that $\underline{p}$ is an eigenvalue of S. Hence, by Equations (10) and (11), U have the eigenvalue of $\cos(-\pi) - i\sin(-\pi) = 1$

However, this contradicts lemma (2.2.1b). Similarly, $E_\pi = 1$ and if $E_{\pi-0} \neq I$ causing an eigenvalue 1 of U

Let $x \in H$ and $y = (1-u)^{-1} x$, then $y \in D(T)$ because $I - U : H \to D(T)$ as shown in proof of lemma (2.2.1b). Hence, from Equation (4), we obtain,

$$Tx = i(i+U)(I-U)^{-1} y = i(i+U)x$$

Recall that $\|Ux\| = \|x\|$, from Equation (9), we have

$$\langle Tx,y\rangle = \langle i(I+U)x,(I-U)x\rangle = i(\langle Ux,x\rangle - \langle x,Ux\rangle)$$
$$= i\left(\langle Ux,x\rangle - \overline{\langle Ux,x\rangle}\right) = -2\operatorname{Im}\langle Ux,x\rangle = 2\int_{-\pi}^{\pi} \sin\frac{\theta}{2}\cos\frac{\theta}{2} d\langle E_\theta x,x\rangle$$

Hence

$$\langle Tx,y\rangle = \int_{-\pi}^{\pi} \sin\frac{\theta}{2}\cos\frac{\theta}{2} d\langle E_\theta x,x\rangle \tag{12}$$

Form the last few lines of the proof of theorem (2.1.2), we recall that (E_θ) is the spectral family of the bounded self-adjoint linear operator S in Equation (10). Hence, E_θ and S commute, so E_θ and U commute by theorem for y. From Equation (6) of the theorem, we can obtain

$$\langle E_\theta y,y\rangle = \langle E_\theta (I-U)x,(I-U)x\rangle = \left\langle (1-U)^* (1-Ut) E_\theta x,x\right\rangle$$
$$= \int \left(1+e^{i\varphi}\right) d\left\langle E_\varphi z,x\right\rangle$$

Where $z = E_\theta x$. Since $E_\varphi E_\theta = E_\varphi$ where $\varphi \leq \theta$ and

$$\left(1+e^{-i\varphi}\right)\left(1+e^{i\varphi}\right) = \left(e^{\frac{i\varphi}{2}} + e^{\frac{-i\varphi}{2}}\right) \Rightarrow 4\cos^2\frac{\varphi}{2}$$

We obtain

$$\langle E_\theta y,y\rangle = 4\int_{-\pi}^{\pi} \cos^2\frac{\varphi}{2} d\left\langle E_\varphi x,x\right\rangle$$

Applying the continuity of E_θ at $\pm\pi$ and the rule for transforming a so called Stieltjes integral we finally have

$$\int_{-\pi}^{\pi}\tan\frac{\theta}{2}d\left\langle E_\varphi y,y\right\rangle=\int_{-\pi}^{\pi}\tan\frac{\theta}{2}\left(4\cos^2\frac{\theta}{2}\right)d\left\langle E_\varphi x,x\right\rangle=4\int\sin\frac{\theta}{2}\cos\frac{\theta}{2}d\left\langle E_\varphi x,x\right\rangle$$

The result is as same as the result in Equation (12).

APPLICATIONS OF UNBOUNDED LINEAR OPERATORS ON QUANTUM MECHANICS

In this section, we shall use notations which are standard in physics some are shown in the table below.

	Notation in physics	Notation used in the preceding chapters
Independent variables	Q	T
Functions	$\phi,\psi,\ldots$	$x,y,\ldots$

Bearing these in mind, we consider the following:

Basic Ideas: States, Observables, and Position Operator

Here, we wish to explain first the basic ideas and concepts of quantum mechanics.
To do this, we consider a single particle which is constrained to one dimension. We consider such system at an arbitrary fixed instant where time t is regarded as a parameter kept constant

State of a system

In classical mechanics, the state of this system at some instant is described by specifying position and velocity of the particle.
In quantum machines, the state of the system is denoted by a function, which is a standard notation in physics. It is a function of a single real variable. Furthermore, we have another standard notation q in place of t (as shown in the table above) which is reserved for time.

In this work, ψ is an element of the Hilbert space $L^2(-\infty,+\infty)$ which suggests a large extent of ψ in physical interpretation. ψ related to the probability that a particle must be found in a given subset say $J\subset R$. Precisely, the probability is

$$\int_J\left|\psi(q)\right|^2dq \tag{1}$$

Hence, we want the particle to be somewhere on the real line R, we now normalize the condition by

$$\|\psi\|^2=\int_{-\infty}^{+\infty}\left|\psi(q)\right|^2dq=1 \tag{2}$$

Our consideration shows that the deterministic description of a state in classical mechanics is now replaced by a probabilistic description of state in quantum mechanics. This situation suggests that state is taken as an element, that's

$$\psi\in L^2(-\infty,+\infty)\ \text{ where }\|\psi\|=1 \tag{3}$$

From Equation (1), $\left|\psi(q)\right|^2$ plays the role of density of probability distribution on $\mathbb{R}$ we therefore obtain the corresponding mean value or expected value by

$$\mu_\psi=\int_{-\infty}^{+\infty}q\left|\psi(q)\right|^2dq \tag{4}$$

Where the variance of the probability distribution is

$$Var_{\psi} = \int_{-\infty}^{+\infty} (q - \mu\psi)^2 \left|\psi(q)\right|^2 dq \tag{5}$$

With the standard deviation given by $Sd_{\psi} = \sqrt{\operatorname{var}\psi} \geq 0$.

Remember that in statistical analysis, μ_{ψ} measures the average value or central location and Var_{ψ} the spread of the distribution.
Consequently, μ_{ψ} characterizes the average ψ position of the particle in a given state ψ.

These notations now bring us to an important point in this work. This is that, we can write Equation (4) in the form

$$\mu_{\psi}(Q) = \langle Q\psi, \psi \rangle = \int_{-\infty}^{+\infty} Q\psi(q)\overline{\psi q}(q)\, dq \tag{6}$$

Where the operator $Q : D(Q) \to L^2(-\infty, +\infty)$ is defined by

$$Q\psi(q) = q\psi(q) \tag{7}$$

(which has a multiplication by the independent variable (q)).

Since we take $\mu_{\psi}(Q)$ as the average position of the particle, Q should be the position operator. Then, $D(Q)$ consists of all $\psi \in L^2(-\infty, +\infty)$ such that $Q_{\psi} \in L^2(-\infty, +\infty)$ where Q is an unbounded self-adjoint operator with domain dense in $L^2(-\infty, +\infty)$. We can now rewrite the variable as

$$Var_{\varphi}(Q) = \langle (Q - \mu I)\psi, \psi \rangle = \int_{-\infty}^{+\infty} \left(Q\psi(q)\overline{\psi q}(q)\right) dq \tag{8}$$

Observable in a system

We know that in physical system, to obtain the state of a system, ψ, some information about quantities that express the properties of the system are needed. These can be observed experimentally. Any of such quantity observed is called an observable. Examples of such observables are position, momentum, and energy.
Now, our concern is to determine the value an observable will assume at a given instant. However, in quantum mechanics, we may ask for the probability that a measurement (an experiment) will produce a value of the observable that lies in a certain interval.
Hence, we define observable (of a physical system at some instant) to be a self-adjoint linear operator $T : D(T) \to L^2(-\infty, +\infty)$.

Analogous to Equations (6) and (8), we define the mean value $\mu_{\psi}(T)$ by

$$\mu_{\psi}(T) = \langle T\psi, \psi \rangle = \int_{-\infty}^{+\infty} T\psi(q)\overline{\psi(q)} dq \tag{9}$$

$$Var_{\psi} = \left\langle (T - \mu I)^2 \psi, \varphi \right\rangle = \int_{-\infty}^{+\infty} (T - \mu I)^2 (q)\overline{\psi(q)} dq \tag{10}$$

And so $\psi(T) = \sqrt{Var(T)} \geq 0$.

Here, $\mu_{\psi}(T)$ characterized the avenge value of the observable T which we can expect in experiment if the system is in a state ψ. The variance $\operatorname{var}\psi(T)$ characterized the spread (i.e., the variability of those values about the mean value)

Application of momentum operator in Heisenberg uncertainty principle

From the previous section, we shall now consider the same physical system with a motivated position operator

$$Q:\mathfrak{D}(Q)\to L^2(-\infty,+\infty)$$
$$\psi\to q\psi$$

We are going to use an important observable – momentum $P\infty$ with a corresponding operator

$$D:\mathfrak{D}(D)\to L^2(-\infty,+\infty)$$
$$\psi\to\frac{h}{2\pi i}\frac{d\psi}{dq}$$

Where h is plank's constant and the domain $\mathfrak{D}(D)\subset L^2(-\infty,+\infty)$ consist of all function $\psi\in L^2(-\infty,+\infty)$ which are absolutely continuous on every compact interval on R and $D\psi\in L^2(-\infty,+\infty)$. A notation of the definition of D is given as follows: By Einstein's mass energy relationship $E=mc^2$ (c is speed of light) and energy E has mass $m={E}/{C^2}$ but since a photon has speed C and $E=hv$(v the frequency), it then has the momentum $p=mc=\frac{hv}{c}=\frac{h}{\wedge}=\frac{h}{2\neq}k$ where $k={2\neq}/{\wedge}$ is a wave length. We should note that the concept of matter waves satisfy this relationships that hold for light waves. Hence, we use the equation above in connection with particles. Now, assuming the state ψ of our physical system to be such that we can apply the classical Fourier integral theorem,

$$\psi(q)=\frac{1}{h}\int_{-\infty}^{+\infty}\psi(q)e^{\left(2\pi i/h\right)}pqdp \tag{4}$$

where

$$\psi(p)=\frac{1}{\sqrt{h}}\int_{-\infty}^{+\infty}\psi(q)e^{\left(-2\pi i/h\right)}pqdq$$

Physically, this can be interpreted as a representation of ψ in terms of function of constant momentum p given by:

$$\psi_q(q)=\varphi(p)e^{ikq}=\varphi(P)e^{\left(2\pi i/h\right)}pq$$

Where $k={2\pi p}/{h}$ by Equation (3) and $\psi(q)$ is the amplitude. The complex conjugate $\bar{\psi}_p$ has a minus sign in the exponent so that

$$\left|\psi_p(q)\right|^2=\psi_p(q)\overline{\psi_p(q)}=\varphi(p)\overline{\varphi_{(p)}}=\left|\varphi(p)\right|^2$$

Since $\left|\varphi_p(q)\right|^2$ is the probability density of the position in state ψ_p, we see that $\left|\varphi(p)\right|^2$ must be proportional to the density of the momentum with the value 1 as the constant of proportionality.

Examining the Equations (4) and (5), they both have same constant ${1}/{\sqrt{h}}$. Hence, by Equation (6), the mean value of the momentum cal it $\bar{\mu}_\psi$, it is given by

$$\bar{\mu}_\psi=\int_{-\infty}^{+\infty}p\left|\varphi(p)\right|^2=\int_{-\infty}^{+\infty}p\varphi(p)\overline{\varphi(p)}dp$$
$$=\int_{-\infty}^{+\infty}p\varphi(p)\frac{1}{\sqrt{h}}\int_{-\infty}^{+\infty}\psi(q)e^{\left(2\pi i/h\right)}pqdqdp$$

Now, by interchanging the order of integration and differentiating the Equation (4) under the integral sign, we obtain

$$\bar{\mu}_\psi=\int_{-\infty}^{+\infty}\overline{\psi(q)}\int_{-\infty}^{+\infty}\psi(p)e^{\left(2\pi i/h\right)}pqdpdq=\int_{-\infty}^{+\infty}\psi(q)\frac{h}{2\pi i}\frac{d\psi(q)}{dq}dq$$

Using Equation (2) and denoting $\bar{\mu}_\psi$ be $\bar{\mu}_\psi(D)$, we establish this equation:

$$\mu_\psi(D) = \langle D\psi, \psi\rangle = \int_{-\infty}^{+\infty} D\psi(q)\overline{\psi(q)}dq$$

This equation really motivates the definition (2) of the momentum operator.

However, our aim is to establish the famous Heisenberg uncertainty principle. To do this, the Heisenberg commutation relation is very paramount in application, so we use an important tool called commutator (C).

Let S and T be among self-adjoint linear operators with domains in the same complex Hilbert space. Then, the operator $C = ST - TS$ is called a commutator of S and T defined on $D(C) = (ST)\cap D(TS)$.

In quantum mechanics, the commutator of the position and momentum operators is of basic importance. By straightforward differentiation, we have,

$$DQ_\psi(q) = \mathfrak{D}(q\psi(q)) = \frac{h}{2\pi i}\left[\psi(q) + q\psi^1(q)\right] = \frac{h}{2\pi i}\psi(q) + QD\psi(q)$$

The Heisenberg commutation relation is therefore established as

$$DQ - QD = \frac{h}{2\neq i}\tilde{I}$$

Where ís identity operator. On the domain

$$\mathfrak{D}(DQ - QD) = \mathfrak{D}(DQ)\cap\mathfrak{D}(QD) \subset L^2(-\infty, +\infty)$$

Theorem 3.1.1 (Commutator)[10]

Let S and T be a self-adjoint linear operators with domain and range in $L^2(-\infty, +\infty)$. Then, $C = ST - TS$ satisfies

$$|\mu_\psi(C)| \le 2Sd_\psi(S)Sd_\psi(T)$$

For every ψ in the domain of C.

Proof:

For simplicity, let $\mu_1 = \mu_\psi(S)$ and $\mu_\psi(T) = \mu_2$ and $S - \mu_1 I = A, T - \mu_2 I = B$, straight forwardly, we calculate $C = ST - TS = AB - BA$.

Since S and T are self-adjoint and μ_1 and μ_2 are inner products then the mean values are real. That is,

$$\mu_\psi(C) = \langle (AB - BA)\psi, \psi\rangle = \langle AB\psi, \psi\rangle - \langle BA\psi, \psi\rangle = \langle B\psi, A\psi\rangle - \langle A\psi, B\psi\rangle$$

which are equal in absolute. Then, by triangle and Schwartz inequalities, we have

$$|\mu_\psi(C)| \le |\langle B\psi, A\psi\rangle| + |\langle A\psi, B\psi\rangle| \le 2\|B\psi\|\|A\psi\|$$

Proving Equation (10). Since B is self-adjoint. Hence, by Equation (10)

$$\|B\psi\| = \left\langle (T - \mu_2 I)^2\psi, \psi\right\rangle^{1/2} = \sqrt{\operatorname{var}\psi(T)} = \operatorname{sd}\psi(T) \text{ it also holds for } \|A\psi\|$$

From Equation (8), we discovered that the commutator of the position and momentum operator is $C = \left(h/_{2\neq i}\right)\tilde{I}$. Hence $|\mu_\psi(C)| = h/_{2\pi}$, then we establish this uncertainty principle as follows

Theorem 3.1.2. (Heisenberg Uncertainty Principle)[11]

For the position operator Q and the momentum operator $S, \operatorname{sd}\psi(D)\operatorname{sd}\psi(Q) \ge \dfrac{h}{4\pi}$

Hence, in physical sense, this inequality (11) means that a person cannot make a simultaneous measurement of position and momentum of a particle with an unlimited accuracy. This is mainly due to the measurement of the system is even a disturbance that changes the state of the system and if the system happened to be small (in the case of an electron), the disturbance becomes noticeable. Thus, any measurement involving an error is caused by the lack of precision of the instrument. Hence, this theorem finally shows that any two observables S and T whose commutator is not a zero operator cannot be measured simultaneously with unlimited precision but the precision is limited in just principle.

Time-independent Schrödinger Equation

In this section, we shall use the analogy between light waves and Broglie's matter waves. We shall derive the fundamental equation called the Schrödinger equation.

Investigating refraction, interference, and other more subtle optical phenomena, we use the wave equation:

$$\psi_{tt} = \gamma^2 \Delta \psi \tag{1}$$

As usual, in connection with stationary wave phenomena, we assume a simple and periodic time dependence, say, of the form:

$$\psi\left(q_1, q_2, q_3, t\right) = \psi\left(q_1, q_2, q_3\right) e^{-iwt} \tag{2}$$

Putting this in Equation (1), we have to drop the exponential factor so that we have the Helmholtz equation called the time-independent wave equation)

$$\Delta\psi + k^2\psi = 0 \tag{3}$$

Where $k = \frac{\omega}{\gamma} = \frac{2\pi v}{\gamma} = \frac{2\pi}{\Lambda}$ and v is the frequency. For Λ, we choose the De Broglie waves length of matter wave, that is

$$\Lambda = \frac{h}{mv} \tag{4}$$

Then, Equation (3) takes the form $\Delta\psi + \frac{8\pi^2 m}{h^2} \cdot \frac{mv^2}{2}\psi = 0$

Let E denote the sum of the Kinetic Energy $mv^2/2$ and the potential energy V that is

$$E = \frac{mv^2}{2} + v$$

Then $\frac{mv^2}{2} E - V$. Then, we have

$$\Delta\psi + \frac{8\pi^2 m}{-h^2}\left(E - V\right)\psi = 0$$

This is the famous time-independent Schrödinger equation, which is fundamental in quantum mechanics. Note that, from Equation (5), we have

$$\left(\frac{-h^2}{8\pi^2 m}\Delta + v\right)\psi = E\psi \tag{6}$$

Suggesting that the possible energy levels of the system will depend on the spectrum of the operator on the left-hand side of Equation (6)

Example 4.1.1 Harmonic Oscillator[12]

Consider the physical system as shown in the figure below which portrays the classical model of a body of mass m attached to the low and of a spring with upper and fixed. In a small vertical motions, we neglect damping and assume the restoring force to be αq that is proportional to the displacement q form the position of static equilibrium them we have the classical differential equation of notion as

$$m\ddot{q} + a \cdot q = 0 \qquad \text{or} \qquad \ddot{q} + \omega_0^2 q = 0$$

Where $\omega_0^2 = a/_m$ and $a = m\omega_0^2$. This is a motion of sine or cosine function. From the restoring force aq we get v the potential energy by integration. Now, we choose a constant of integration so that V is zero at $q = 0$. We have $V = a\,q^2/_2 = m\omega_0^2\,q^2/_2$.

Recall the Equation (5) above of Schrödinger equation of the harmonic oscillator, which we shall now put as

$$\psi'' + \frac{8\pi^2 m}{h^2}\left(E - \frac{1}{2} m\omega_0^2 q^2\right)\psi = 0 \tag{1}$$

Setting

$$\bar{\lambda} = \frac{4\pi}{\omega_0 h} E \tag{2}$$

And multiplying Equation (1) with $b^2 = h/_{2\pi}\, m\omega_0$ we have

$$b^{2\psi=0}\psi''\left[\bar{\lambda} - \left(\frac{q}{b}\right)\right]^2$$

Then, introducing $S = q/b$ as a new independent variable and writing $\psi(q) = \bar{\psi}(S)$, we have

$$\frac{d^2\bar{\psi}}{dS^2} + \left(\bar{\lambda} - S^2\right)\bar{\psi} = 0 \tag{3}$$

Solving the Equation (9) in $L^2(-\infty, +\infty)$, we substitute $\bar{\psi}(S) = e^{-S^2/_2} V(S)$ in Equation (3) and omitting the exponential factor

$$\frac{V}{ds^2} - 2S\frac{dv}{ds} + \left(\bar{\lambda} - 1\right)V = 0 \tag{4}$$

For $H_n = 2n+1, n = (0,1,2,\ldots)$

This becomes identical with Equation (3) except for the notation. Hence, the Hermite polynomial H_n is the solution of the equation. The first few of these function H_n formed are represented in the diagram below with respect to their set of orthonormal eigenfunction(e_n) satisfying Equation (3) above. Since $V = \omega_0/_{2\pi}$, then for eigenvalue $\bar{\lambda}$, these corresponding to the energy levels

$$E_n = \frac{w_0 h}{4\neq}(2n+1) = hV(n+1/2)$$

Then, for the first four eigenfunctions e_n, we have energy levels $hv/_2, 3hv/_2, 5hv/_2$, and $7hv/_2$ which give the graph as in Figures 1-3 below:

The so-called half integral multiples of energy quantum hv are characteristic of the oscillator.

The zero point energy is now $hv/_2$ instead of 0 as was assumed before by max plank in quantum theory the number n specifies the energy level and is named the principal quantum number of the harmonic oscillator.

Hamilton operator

In classical mechanics, one can base the investigation of a conservative system of particles on the Hamilton function of the system; this is the total energy

$$H = E_{kin} + v \tag{1}$$

E_{kin} = kinectic energy and V = potential energy are expressed in terms of position coordinates and momentum coordinates. Assuming that the system has n degrees of freedom, one has n position coordinates, $q_1,\ldots,q_n$ and n momentum coordinates, $p_1 p_2 \cdots p_n$. In the quantum mechanical treatment of the system, we also determine $H\left(p_1,\ldots,p_n,q_1,\ldots,q_n\right)$. Then, we replace each p_j by the momentum separator

$$D_j : \mathsf{D}(D) \rightarrow L^2\left(\left|R^n\right.\right)$$

$$\psi \rightarrow \frac{h}{2\pi i}\frac{\partial\psi}{\partial q_1}$$

Where $\mathsf{D}\left(D_j\right) \subset L^2\left(R^n\right)$. Furthermore, we replace each q_j by the position operator

$$Q_j : \mathsf{D}\left(Q_j\right) \rightarrow L^2\left(\left|R^n\right.\right)$$

$$\psi \rightarrow q_j\psi$$

Where $\mathsf{D}(Q) \subset L^2\left(R^n\right)$, from the above Hamilton function H, we then obtain the Hamilton operator, which we denote by $\mathsf{H}\left(D_1,\ldots,D_n,Q_1,\ldots,Q_n\right)$ this is $H\left(p_1,\ldots,p_n,q_1,\ldots,q_n\right)$ where p_j is replaced by D_j and q_j replaced by Q_j. By definition H is assumed to be self-adjoint.

This process of replacement is called the quantization rule. Note that the process is not unique, because the multiplication is commutative only for numbers but not for operators. This, therefore, becomes a deficiency (or weaknesses) of quantum mechanics.

Now, from Equation (6) above, we can rewrite the equation using Hamilton operator H. In fact, the kinetic energy of a particle of mass m in space is

$$\frac{m}{2}\left|v^2\right| = \frac{m}{2}\left(V_1^2 + V_2^2 + V_3^2\right) = \frac{1}{2m}\left(P_1^2 + P_2^2 + P_3^2\right)$$

By the quantization rule, we produce

$$\frac{1}{2m}\sum_{j=1}^{3} D_j^2 = \frac{1}{2m}\left(\frac{h}{2\pi i}\right)^2 \sum_{j=1}^{3}\frac{\partial^2}{\partial qj^2} = -\frac{h^2}{8\pi^2 m}\Delta$$

Hence, Equation (6) can be written as

$$\mathsf{H}\psi = \lambda\psi \tag{4}$$

Where $\lambda = E$ the energy. If λ is in the resolvent set of H, the resolvent of H exists and Equation (4) has only the trivial solution, considered in $L^2\left(R^n\right)$. If λ is in the point spectrum $\sigma_p(\mathsf{H})$, then Equation (4) has non-trivial solution $\psi \in L^2\left(R^n\right)$. If $\lambda \in \sigma_c(\mathsf{H})$ the continuous spectrum of H, the Equation (4) has no solution $\psi \in L^2\left(\left|R^n\right.\right)$ where $\psi \neq 0$ so Equation (4) may have nonzero solutions that are not in $L^2\left(R^n\right)$ but only depends on the parameter with respect to which we can perform integration to obtain $\psi \in L^2\left(R^n\right)$.

Since H is an extension of original operator, the function under consideration is the domain of the extended operator. Hence, this process may be explained in terms of the following physical system. That is, considering a free particle of mass m on $(-\infty,+\infty)$. The Hamilton function is $H(p,q) = \frac{1}{2m}p$ so that we obtain the Hamilton operator

$$\mathsf{H}(D,Q) = \frac{1}{2m}D^2 = \frac{h^2}{8\neq^2 m}\frac{d^2}{dq^2} \ni$$

Equation (4) becomes

$$\mathsf{H}\psi = -\frac{h^2}{8\pi^2 m}\psi'' = \lambda\psi \tag{5}$$

Where $\lambda = E$ is the energy. Then, solution is given by

$$\eta(q) = e^{-ikq} \tag{6}$$

Where k is related to the energy by

$$\lambda = E = \frac{h^2 k^2}{8\pi^2 m}$$

These functions η can be used to represent any $\psi \in L^2(-\infty, +\infty)$ as wave packet in the form

$$\psi(q) = \frac{1}{\sqrt{2\pi}} \lim_{a\to\infty} \int_{-a}^{a} \psi(k) e^{-ikq} dk \tag{7a}$$

Where,

$$\psi(k) = \frac{1}{\sqrt{2\pi}} \lim_{a\to\infty} \int_{-b}^{b} \psi(k) e^{ikq} dq \tag{7b}$$

The two of Equation (7) with the limit in the mean is called the Fourier Plancherel theorem. The extension of this consideration to a free particle of mass in three dimensional space is as follows. Now, instead of Equation (5), we obtain

$$\mathsf{H}\psi = \frac{h^2}{8\pi^2 m}\Delta\psi = \lambda\psi \tag{8}$$

which has the solutions of plane waves as

$$\eta(q) = e^{-ikq} \tag{9a}$$

Where $q = (q_1, q_2, q_3), k = (k_1, k_2, k_3)$ and $k \cdot q = k_1 \cdot q_1 + k_2 \cdot q_2 + k_3 \cdot q_3$ the energy becomes

$$\lambda = E = \frac{h^2}{8\pi^2 m} k \cdot k \tag{9b}$$

In general, for $\psi \in L^2\left(|R^3\right)$, the Fourier Plancherel theorem gives:

$$\psi(q) = \frac{1}{(2\pi)^{3/2}} \int_{|R^3} \varphi(R) e^{-ik\cdot q} dq \tag{10}$$

Where the integrals should again be understood as the limit in the mean of the corresponding integrals over finite regions in three space.

Example 4.2.1 (**Harmonic Oscillator**)[12] Given a Hamilton function of the harmonic oscillator; $H = \frac{1}{2m}p^2 + \frac{1}{2}mw_0^2 q^2$ then the Hamilton operator is

$$\mathsf{H} = \frac{w_0^2}{2}\left({}^{1}\!/_{a^1} D^2 + a^2 Q^2 \right), (a = mw_0)$$

Simplifying the equation, we have

$$A = \beta\left(aQ - {}^{i}\!/_{a} D\right), \left(\beta^2 = {}^{\pi}\!/_{h}\right)$$

Now, the Hilbert adjoint operator is $A = B\left(\alpha Q - {}^{i}\!/_{a} D\right)$ such that,

$$A = {}^{\pi}\!/_{h}\left(a^2 Q^2 + {}^{1}\!/_{a^2} D^2 - {}^{h}\!/_{2\pi} I\right) \tag{14a}$$

$$AA^* = \pi/_h\left(aQ^2 + 1/_{a^2}D - h/_{2\pi}I\right) \tag{14b}$$

Hence $AA^* - A^*A = I$

From Equations (14a) and (11)

$$\mathsf{H} = \frac{\omega_0 h}{2\pi}\left(A^*A + 1/_2 I\right)$$

We now show that any eigenvalue λ of H must equal one of the values given by Equation 12 of the previous section.
Let λ be an eigenvalue of H and ψ an Eigen function then $\psi \neq 0$ and $\mathsf{H}\psi = \lambda\psi$

By Equation (16)

$$A^*A\psi = \lambda\psi \text{ where } \bar{\lambda} = \frac{2\pi\lambda}{\omega_0 h} - 1/_2 \tag{17}$$

Applying A, we have

$$AA^*(A\psi) = \lambda A\psi$$

On the left, $AA^* = A^*A + I$ by Equation (15). Hence

$$A^*A(A\psi) + (\bar{\lambda} - j)A^j\psi \tag{18}$$

Where $A^j\psi = 0$ for sufficiently large j. This is because otherwise, taking the inner product by $A'\psi$ on both sides of Equation (18), we obtain $\forall j$

$$\langle A'\psi, A^*A(A'\psi)\rangle = \langle A^{j+1}\psi, A^{i+1}\psi\rangle = (\bar{\lambda} - j)\langle A^j\psi, A^j\psi\rangle$$

That is $\bar{\lambda} - j = \dfrac{\left\|A^{j+1}\psi\right\|^2}{\left\|A^j\psi\right\|} \geq 0, \forall j$

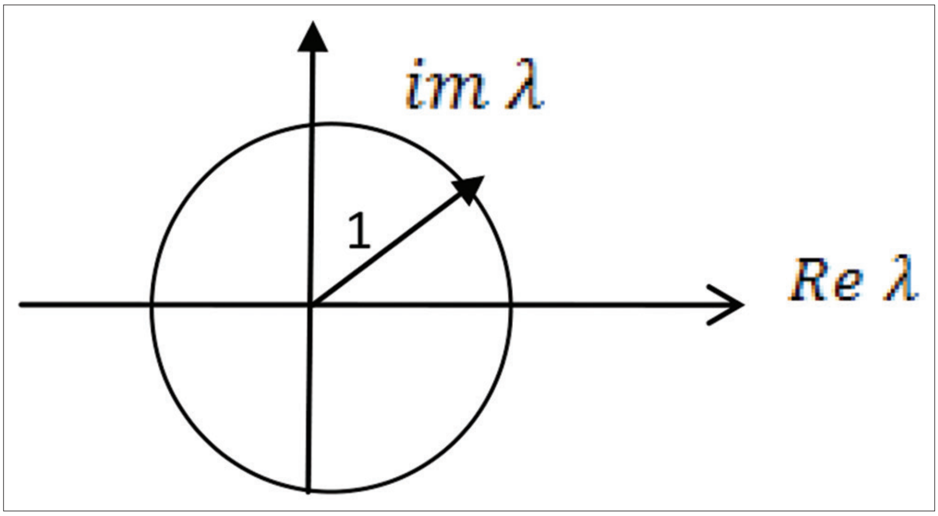

Figure 1: Unit Circle in the Complex Plane

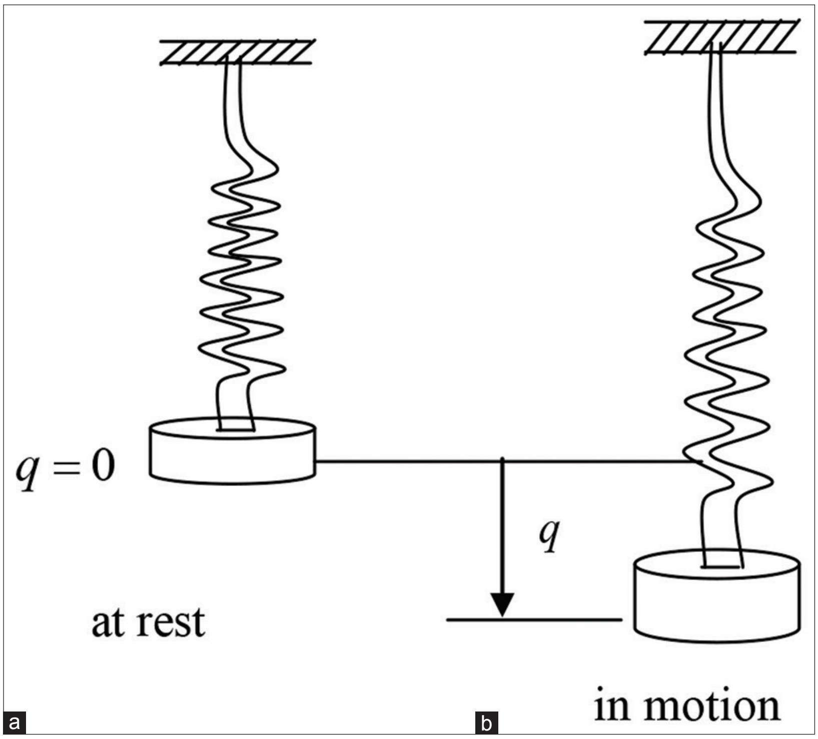

Figure 2: Body on a spring

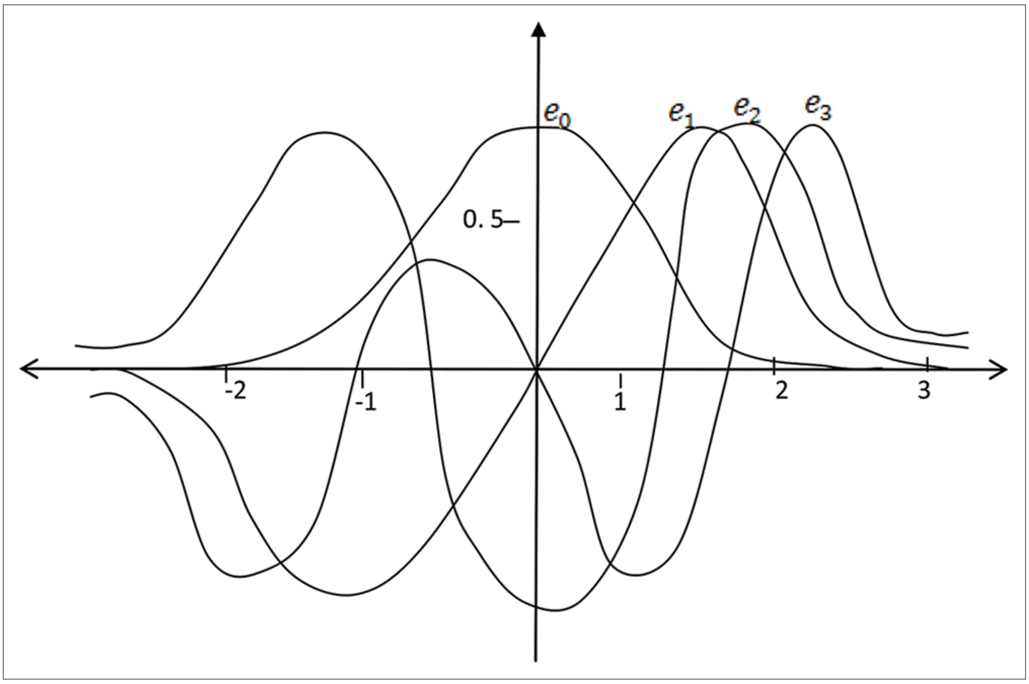

Figure 3: Shows the first four Eigen functions e_0, e_1, e_2, e_3 of the harmonic oscillator corresponding to the energy levels $hv/2, 3hv/2, 5hv/2, 7hv/2$ where $n = 0,1,2,\ldots$

This cannot hold since $\bar{\lambda}$ is a certain number hence there is an $n \in N \ni A^n\psi \neq 0$ but $A^j = 0$ for $j > n$ in particular $A^{n+1}\psi = 0$ from $j = n$, we thus obtain from this and Equation (17), since $\omega_0 = 2\pi V$

$$\lambda - \frac{\omega_0 h}{2\pi}\left(n + 1/2\right) = hv\left(n + 1/2\right)$$

Corresponding with Equation 12 of example (4.1.1)

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