

Time-Evolution as an Operator in Hilbert Spaces with Applications in Quantum Mechanics

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ABSTRACT: *The main aim of this article is to present the time-evolution as the unitary and self-adjoint operators on Hilbert spaces and to describe its application in the development of quantum mechanics. The initial value problems associated with the quantum mechanical Schrodinger equation, $i\frac{d\psi(t)}{dt} = H\psi(t)$ in the Hilbert space is solved by the use of time-evolution. The importance of time-evolution is also seen as the operation of turning machine in quantum mechanics, which is regarded as the time-evolution of the machine control state. Time-evolution of a quantum mechanical system is observed to be unitary and self-adjoint operators of Hilbert space, since it corresponds to an observable, specifically energy position and momentum. It was observed that time-evolution of a quantum mechanical system is generated by a self-adjoint operator, called Hamiltonian, $\hat{H} = \hat{K} + \hat{V}$, expressed by the Schrodinger equation, above.*

Keywords: *Time-evolution, self-adjoint operator, unitary operator, Hamiltonian operator, observable, commutator relation, Quantum mechanics.*

1. INTRODUCTION

Time is the dimension in which events can be ordered from the passed through the present and into the future [3]. It can also be explained as the measure of duration of events and the intervals between them. Evolution can be explained as the process of transformation or growth. Based on these definitions, time-evolution can be explained as the change of state due to the passage of time, applicable to the system with interval state (also called stateful system). In this formulation, time is not required to be a continuous parameter, but a discrete or even finite.

In classical physics, time-evolution of a collection of rigid bodies is controlled by the principle of classical mechanics. In their most rudimentary form, these principles express on the relationship between forces acting on the bodies and their acceleration given by Newton's law of motion. These principles can also be equivalently expressed more abstractly by Hamiltonian mechanics.

The concepts of time-evolution may be applicable to the stateful system as well. For example, the operator of a turning machine can be regarded as the time evolution of the machine control

state. In this perspective, time is discrete. The stateful system of operators often has dual description in terms of states or in terms of observable values which constitute quantum mechanics. In such system, time-evolution can also be called the change in observable values. This is particularly important in quantum mechanics where the Schrodinger picture and Heisenberg picture are equivalent description of the time-evolution.

The time evolution of the state vector $|\psi(t)\rangle$ of a physical system is governed by the Schrödinger equation. $i\hbar \frac{d|\psi(t)\rangle}{dt} = H(t)|\psi(t)\rangle$, where $H(t)$ is the observable corresponding to the classical Hamiltonian of the system. The evolution of a quantum system is controlled by the Schrödinger equation, $\frac{\partial f}{\partial t} = -iHf$, with solution $f(x,t) = e^{-iHt}f(x,0)$. The total energy $\langle Hf, f \rangle$ of the system is divided between the kinetic energy $\langle -\Delta f, f \rangle$ and the potential energy $\langle Vf, f \rangle$ [11]. Time-evolution is aimed at looking at the initial value problem associated with the Schrödinger equation $i \frac{d\psi(t)}{dt} = R\psi(t)$ in the Hilbert space. If R is one-dimensional, the solution is given by $\psi(t) = e^{-itR}\psi(0)$, where R is a real number. Moreover, the unitary operator $\langle U(t)\psi, RU(t)\psi \rangle = \langle U(t)\psi, U(t)R\psi \rangle = \langle \psi, R\psi \rangle$,

shows that the expectations of the real number R are time-independent which corresponds to the conservation of energy [10].

On the other hand, the generator of the time-evolution of a quantum mechanical system is observed to be always an operator on Hilbert space (self-adjoint operator), since it corresponds to an observable (energy). Moreover, there should be a one-one correspondence between the unitary group and its generators. This fact is supported by the Stone's theorem.

The time-evolution as an operator (unitary operator) in Hilbert space can be explained through the use of the solution of Schrödinger equation that can be used for this explanation can be written in the form $|\psi(t)\rangle = e^{\{-iRt\}}|\psi(0)\rangle$.

The operator $e^{\{-iRt\}}$ is a unitary operator and is called the time-evolution operator, since it takes a state at t' to time $t+t'$. By the $*$ -homomorphism property of the functional calculus, the operator $U = e^{-iHt/\hbar}$ is a unitary operator. It is the time-evolution operator or propagator of a closed quantum system. If the Hamiltonian is time-independent, the unitary operator, $[U(t)]$ form a one parameter unitary group [10] [5].

Any symmetry of the system is represented by a unitary operator on its Hilbert space. The symmetry here is time-translation invariance. This is because we expect symmetry to have no effect on the transition probabilities between various states, which means it should preserve the inner product on the Hilbert space and this is precisely what a unitary operator does. This

shows that the unitary operator can be thought of as the generalization to Hilbert space of orthogonal transformation (i.e., rotation).

To observe more of this concepts, let us consider a system with state space X for which evolution is deterministic and reversible. Let us also suppose that time is a parameter that ranges over the set of real number \mathcal{R} . The time-evolution is expressed as a family of bijective state transformations

$$F_{t,s}: X \rightarrow X \text{ for all } t, s \in \mathcal{R}$$

Where $F_{t,s}$ is the state of the system at time t , whose state at time s is X . This leads to the existence of the following identity operator

$$(F_{t,s}(X)) = F_{s,t}(X)$$

In some contexts in mathematical physics, the mapping, $F_{t,s}$ are called the propagation operators. In quantum mechanics, the propagators are usually unitary operators or self-adjoint operators on Hilbert space which can be expressed as time-ordered exponentials of the combined Hamiltonian operator [6] [1].

2. PRELIMINARY

Definition 1. Time Evolution: Time-evolution is referred to as the change of state due to the passage of time, applicable to the system with internal state. If Ψ is the wavefunction for a physical system of an initial time and the system is free of external interactions, then the evolution of time of the wavefunction is given by $H\Psi = i\hbar \frac{\partial \Psi}{\partial t}$, where H is the Hamiltonian.

Definition 2. Time Evolution for Conservative Systems: A physical system is conservative if its Hamiltonian does not depend explicitly on time. In quantum mechanics, as well as, in classical mechanics, the most important of such an observation is the conservation of energy. The time evolution of the system that was initially in the state $|\Psi(t_0)\rangle$ is using the following steps:

- (i) Expand state vector $|\Psi(t_0)\rangle$ in the basis of eigenvector of H , i.e.

$$|\Psi(t_0)\rangle = \sum_n \sum_k a_{nk}(t_0) |\varphi_{nk}\rangle, \text{ where } a_{nk}(t_0) = \langle \varphi_{n,k} | \Psi(t_0) \rangle.$$

(ii) To obtain $|\psi(t)\rangle$ for $t > t_0$, multiply each coefficient $a_{n,k}(t_0)$ by $e^{-iE_n(t-t_0)/\hbar}$ where

E_n is the eigenvalue of H associated with the state $|a_{n,k}\rangle$, meaning

$$|\psi(t)\rangle = \sum_n \sum_k a_{n,k}(t_0) e^{-iE_n(t-t_0)/\hbar} |\phi_{n,k}\rangle. \text{ This step can be}$$

generalised to the case of $\delta_c(H) \cdot S|\psi(t)\rangle = \sum_k \int a_k(E, t_0) e^{-iE_n(t-t_0)/\hbar} |\phi_{E,k}\rangle dE$. The

eigenstates of H are called stationary states [11].

Definition 2. Time- Evolution for the Mean Value systems: Let $|\psi(t)\rangle$ be the normalised ket describing the time- evolution of a physical system. The time- evolution of the mean value of observable, A is governed by the equation $\frac{d\langle A \rangle}{dt} = \frac{1}{i\hbar} \langle [A, H(t)] \rangle$. If A does not depend

explicitly on time, we have $\frac{d\langle A \rangle}{dt} = \frac{1}{i\hbar} \langle [A, H(t)] \rangle$. By definition, a constant of motion is an observable, A , that does not depend explicitly on time and commutes with the Hamiltonian H .

In this case, $\frac{d\langle A \rangle}{dt} = 0$ [11].

Definition 3. Self-Adjoint and unitary operators: A bounded linear operator $T: H \rightarrow H$ on a Hilbert space H is said to be;

i. self-adjoint if $T = T^*$ i.e. $(Tx, y) = (x, Ty)$ for all $x, y \in H$

ii. Unitary if T is bijective if $T^* = T^{-1}$.

Definition 4. Quantum mechanics: Quantum mechanics is a branch of mechanics (science of movement and force) that deals with the mathematical description of the motion on interaction with subatomic particles. It describes the motion at every level of microscopic particles [6].

Definition 5. Observables: These are measurable operators, where the property of the system state can be determined by some sequence of physical operators. They are quantities whose values can be measured, for example, momentum, position and energy operators [5].

Definition 6. Hamiltonian operator in Quantum Mechanics: In quantum mechanics, Hamiltonian is the operator corresponding to the total energy of the system. This operator is usually denoted by H . Its spectrum is the set of possible outcome when one measure of the total energy of the system. Due to its close relation to the time-evolution of a system, it is of fundamental importance in most formulation of quantum theory [4].

Hamiltonian as an operator in quantum mechanics is used to explain the Schrodinger equation. It is commonly expressed as the sum of kinetic energies of all the particles and the potential energy of the particles associated with the system. It is given in the form, $\hat{H} = \hat{K} + \hat{V}$

, where $\hat{V} = V = V(r, t)$ is the potential energy operator and $\hat{K} = \frac{\hat{p} \cdot \hat{p}}{2m} = \frac{\hat{p}^2}{2m} = \frac{-\hbar^2}{2m} \nabla^2$ is the kinetic energy operator in which m is the mass of the particles involved. The dot denotes the dot product of the vectors and $\hat{p} = -i\hbar \nabla$ is the momentum operator, where ∇ is the gradient operator. The dot product of ∇ with itself is the laplacian ∇^2

. In three dimensions using Cartesian coordinate, the laplace operator is

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}.$$

When these forms are combined together, it yields the formula used in the Schrödinger

equation $\hat{H} = \hat{K} + \hat{V} = \frac{\hat{p} \cdot \hat{p}}{2m} + V(r, t) = -\frac{\hbar^2}{2m} \nabla^2 + V(r, t)$, which allows one to apply the

Hamiltonian to system described by a wave function $\psi(r, t)$. this is the approach commonly taken in introductory treatment of quantum mechanics, using the formalism of Schrodinger's wave mechanics [6] [2].

Definition 7. Schrödinger Equation: The Hamiltonian operator generates the time-evolution of quantum states. If $|\psi(t)\rangle$ is the state of function at time, t , then $H |\psi(t)\rangle = i\hbar \frac{\partial \psi}{\partial t} |\psi(t)\rangle$. This is called the Schrödinger equation. It takes the same form as the Hamilton-Jacobian equation,

$$\frac{\hbar^2}{2m\psi} (\nabla \psi)^2 - U\psi = \frac{\hbar}{i} \frac{\partial \psi}{\partial t}$$

which is one of the reasons it is called the Hamiltonian. Given

the state at some initial time ($t = 0$), we can solve it to obtain the state at any subsequent time.

In particular, if Hamiltonian is independent of time, then $|\psi(t)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle$ [11].

Definition 8. Schrodinger Picture: In Physics, the Schrodinger Picture is a formation of quantum mechanics in which the state vectors evolve in time, but the operators (observables) are constant with respect to time. In the Schrodinger Picture, the state of a system evolves with time. The evolution for a closed quantum system is brought about by a unitary operator, the time evolution operator [8] [9].

Definition 9. Heseinberg Picture: In Physics, the Heseinberg Picture is a formation of quantum mechanics in which the operators (observables) incorporate a dependency on time, but the state vectors are time –independent. In Heseinberg Picture of quantum mechanics, the vectors $|\varphi\rangle$ do not change with time while the observable B satisfy $\frac{d}{dt}B(t) = \frac{i}{\hbar}[H, B(t)] + \frac{\partial B(t)}{\partial t}$, where H is the Hamiltonian and $[.,.]$ indicates the computation of two operators (H and B).

Definition 11. The * –homomorphism: This is the time-evolution operator or propagator of a closed quantum system. It can also be explained using the idea of c*-algebra as seen below: Let A and B be two c*-algebras. Then the bounded linear map $\pi: A \rightarrow B$, between A and B is called a * – homomorphism if

- (i) For x and y in A, $\pi(xy) = \pi(x)\pi(y)$
- (ii) For x in A, $\pi(x^*) = \pi(x)^*$

This is also applicable to B [1].

Definition 12. Turning Machine: This is one of the aspects of quantum mechanics where time-evolution (unitary operator) play its role in its performance. It is a hypothetical device that manipulates symbols on a strip of tape according to a table of rules. It helps physicists in taking the accurate measurement10of length of moving machines in physics laboratories. It also assists the computer scientists to understand the limits of mechanical computations [10].

Definition 13. Commutator Relation: This is the basic relation between conjugate qualities (quantities which are related by definition such that one is the Fourier transform of another). For instance, $[x, px] = i\hbar$ between the position x and momentum px in the direction x of a point particle in one-dimension, where $[x, px] = xpx - pxx$ is the commutator of x and px , i is the imaginary unit and \hbar is the reduced plank's constant i.e $\hbar = \frac{h}{2\pi}$. It may look different than in the Schrodinger picture because of the time dependent of operator. For example, consider the operators $x(t_1)$, $x(t_2)$, $p(t_1)$ and $p(t_2)$. The time- evolution of these operators depend on the Hamiltonian of the system in quantum mechanics [8] [9].

3. BASIC THEOREMS

Here, we use this avenue to look at the initial value problem associated with the Schrödinger equation in the Hilbert space, \mathfrak{H} . If \mathfrak{H} is one- dimensional, the solution is given by $|\psi(t)\rangle = e^{-itA}|\psi(0)\rangle$, where A is a real number. Our hope is that this formula also applies in the general case and that we can reconstruct a one-parameter unitary group $U(t)$ from its generator A through $U(t) = \exp(-itA)$. we first investigate the family of operator $\exp(-itA)$

Theorem 1: Let A be self-adjoint and let $U(t) = \exp(-itA)$. then

i $U(t)$ is a strongly continuous one-parameter unitary group;

ii The $\lim_{t \rightarrow 0} \frac{1}{t}(U(t)\psi - \psi)$ exists if and only if $\psi \in D(A)$ and in case

$\lim_{t \rightarrow 0} \frac{1}{t}(U(t)\psi - \psi) = -iA\psi$. And on the other hand, the generator of the time-evolution of a quantum mechanical system should always be a self-adjoint operator since it corresponds to an observable (energy). Moreover, there should be a one-one correspondence between the unitary group and its generator. This is ensured by the Stone's theorem [10].

Theorem 2: Stone's theorem. Let $U(t)$ be a weakly continuous one-parameter unitary group. Then its generator R is self-adjoint and $U(t) = e^{-itR}$.

Now we have seen that the time-evolution of a quantum mechanical system is generated by a self-adjoint operator (Hilbert space operator), called Hamiltonian and is expressed and governed by a linear ordinary differential equation, the Schrodinger equation,

$$i \frac{d}{dt} \psi(t) = H\psi(t). \quad [10].$$

Remark 1: Unitary Relation of Position and Momentum Operators

The position and momentum operators are unitarily equivalent with the unitary operator being given explicitly by the Fourier transform. Thus, they have the same spectrum. In physical sense, the force p acting on momentum space wavefunction is the same as position space wavefunction. This resulted in the Heisenberg Uncertainty Principle.

Theorem 3: Heisenberg Uncertainty principle. Let H be a Hilbert space and let $(D(T), T)$ and $(D(S), S)$ be self-adjoint operators on H . Also, let $v \in D(T) \cap D(S)$ be such that $Tv, Sv \in D(T) \cap D(S)$. Again let μ_T, μ_S be the spectral measure for v with respect to T and S . Furthermore, let $\delta_T^2 = \int_{\mathbb{R}} (x - t_0)^2 d_{\mu_T}(x)$ and $\delta_S^2 = \int_{\mathbb{R}} (x - s_0)^2 d_{\mu_S}(x)$,

where t_0, s_0 are the average of μ_T and μ_S . Then we have

$$\delta_T^2 \delta_S^2 \geq \frac{1}{4} (\langle i\omega, v \rangle)^2,$$

where $\omega = TSv - STv = [T, S]v$ [7].

Remark 2: It was observed that we can use the idea of the principle above to explain the uncertainty of the result of measurements of two observables of quantum mechanics. To achieve that, let us consider two observables a and b , with corresponding operators \hat{a} and \hat{b} .

Let ψ be a vector such that $(\hat{a}\hat{b}-\hat{b}\hat{a})\psi$ makes sense. The uncertainties of the result of measurement of a and b in the state ψ are just

$$\Delta a = \Delta_{\psi} a = \sqrt{\delta_{\psi} a} = \|\hat{a}\psi - \bar{a}_{\psi}\psi\|$$

$$\Delta b = \Delta_{\psi} b = \sqrt{\delta_{\psi} b} = \|\hat{b}\psi - \bar{b}_{\psi}\psi\|$$

We have $\Delta a \Delta b \geq \frac{1}{2} |((\hat{a}\hat{b}-\hat{b}\hat{a})\psi, \psi)|$. Indeed let $\hat{a}_1 = a - \bar{a}_{\psi}I$, $\hat{b}_1 = b - \bar{b}_{\psi}I$. Then $\hat{a}_1\hat{b}_1 - \hat{b}_1\hat{a}_1$.

Hence

$$\begin{aligned} |((\hat{a}\hat{b}-\hat{b}\hat{a})\psi, \psi)| &= |((\hat{a}_1\hat{b}_1 - \hat{b}_1\hat{a}_1)\psi, \psi)| \\ &= |(\hat{a}_1\hat{b}_1\psi, \psi) - (\hat{b}_1\hat{a}_1\psi, \psi)| \\ &= |(\hat{b}_1\psi, \hat{a}_1\psi) - (\hat{a}_1\psi, \hat{b}_1\psi)| \\ &= 2\text{Im}(\hat{a}_1\psi, \hat{b}_1\psi) \leq 2|(\hat{a}_1\psi, \hat{b}_1\psi)| \leq 2\|\hat{a}_1\psi\|\|\hat{b}_1\psi\| \\ &= 2\|\hat{a}\psi - \bar{a}_{\psi}\psi\|\|\hat{b}\psi - \bar{b}_{\psi}\psi\| \\ &= 2\Delta a \Delta b. \end{aligned}$$

We say that the observables a and b are convergent if $\hat{a}\hat{b}-\hat{b}\hat{a} = \frac{h}{i}I$. In this case, the right hand part of the Heisenberg commutation relation $[\hat{p}_k, \hat{q}_j] = \frac{h}{i}I[\hat{p}_k, \hat{q}_j] = 0, k \neq j$, and

$$\Delta \hat{p}_k \Delta \hat{q}_j \geq \frac{h}{2}.$$

4. RESULTS

Remark 3: It was deduced from the work that the Hamiltonian operator generates the time-evolution of quantum states by the Schrodinger equation, $H|\psi(t)\rangle = i\hbar \frac{\partial \psi(t)}{\partial t}$. Bearing in mind the commutator relation and considering the one-dimensional harmonic oscillator $H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}$, the time- evolution of the position and momentum operators is given by

$$\frac{d}{dt}x(t) = \frac{i}{\hbar}[H, x(t)] = \frac{p}{m}, \quad \frac{d}{dt}p(t) = \frac{i}{\hbar}[H, p(t)] = -m\omega^2 x.$$

Differentiating once more and solving with proper initial condition,

$$\dot{x}(0) = \frac{p^0}{m}$$

$p(0) = -m\omega^2 x$, leads to

$$x(t) = x_0 \cos(\omega t) + \frac{p^0}{\omega m} \sin(\omega t)$$

$$p(t) = p_0 \cos(\omega t) - m\omega x_0 \sin(\omega t)$$

Direct computation yields more general commutator relation as

$$\begin{aligned} [x(t_1), x(t_2)] &= \frac{i\hbar}{m\omega} \sin(\omega t_2 - \omega t_1) \\ [p(t_1), p(t_2)] &= i\hbar m\omega \cos(\omega t_2 - \omega t_1) \\ [x(t_1), p(t_2)] &= i\hbar \cos(\omega t_2 - \omega t_1) \end{aligned}$$

For $t_1 = t_2$ we simply recovers the standard canonical commutator relations valid in all pictures.

Remark 4: It was also deduced that the position and momentum operators in quantum mechanics are equal with the same spectrum as well as the force acting on their wavefunction. This is supported by theorem 3.

Remark 5: Theorems 1 and 2 indicate that the time-evolution of a quantum mechanical system is always a self-adjoint operator since it corresponds to an observable (energy). Furthermore, there is a one-one correspondence between the unitary group and its generator showing that it is also unitary.

Remark 6: One of the aspects of quantum mechanics where time-evolution (unitary operator) play its role in its performance is ‘Turning Machine’. It helps physicists in taking correct measurement and can be adopted by the computer scientists to simulate the logic of an computer algorithm. It is also useful in explaining the functions of central processing unit (CPU) of a computer. The limits of mechanical computations is also understood by the system.

5. CONCLUSION

From the discussion above, it was clearly observed that time-evolution has played a significant role in the formation of quantum mechanical systems as being both the unitary and self-adjoint operators of Hilbert space. This is so since it corresponds to the observables (energy position and momentum) of quantum mechanics. The idea of commutator relation and the one-dimensional harmonic oscillator $H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}$, facilitate the time- evolution of the position and momentum operators as $\frac{d}{dt}x(t) = \frac{p}{m}$ and $\frac{d}{dt}p(t) = -m\omega^2 x$, generated from $\frac{i}{\hbar}[H, x(t)]$ and $\frac{i}{\hbar}[H, p(t)]$. The time-evolution of a quantum mechanical system is also generated by a self-adjoint operator, called Hamiltonian, $\hat{H} = \hat{K} + \hat{V} = -\frac{\hbar^2}{2m} \nabla^2 + V(x)$.

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