Approximation Methods for the Solution of Quantum Evolution Equations at the Zero Fluctuation Limit

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Abstract: This paper is focused on the solution of a univariate quantum dynamical system that can be treated through the dynamics of expectation values of the position and momentum operators. This goal is realised by using the fluctuationlessness theorem. The concerned equations are matrix equations and derived using the wave function of the Schrödinger equation. The quality of the obtained approximated solution is tested by comparing it with the real solution for different $n$ values.

Key–Words: Quantum Dynamical System, Schrödinger Equation, Expectation Value, Fluctuationlessness, Hilbert Space, Operator, Ordinary Differential Equations

1 Introduction

Two time variant square matrices are at the focus of the work: position matrix $\mathbf{X}(t)$ and momentum matrix $\mathbf{P}(t)$. They are assumed to be of type $n \times n$ and satisfy the following set of equations

$$\dot{\mathbf{X}}(t) = \mathbf{P}(t)$$

$$\dot{\mathbf{P}}(t) = f(\mathbf{X}(t))$$

where $f$ symbolizes a univariate function. The above equations are called “Evolution Equations”[1]. The initial values of the position and momentum matrices correspond to the initial state of the quantum system under consideration.

$$\mathbf{X}(0) = \mathbf{A}, \quad \mathbf{P}(0) = \mathbf{B}$$

Although these are ordinary differential equations and can be numerically solved via standing approximation methods, it becomes very important to develop new approximation tools which are based on the physical and conceptual specification of the problem under consideration. To this end, a novel approach developed by Demiralp[2] and based on the fluctuationlessness theorem is standing at the horizon as a candidate of numerical ODE solver for these kinds of problems.

In order to get the evolution equations, we will first deal with the Schrödinger equation. It is a wave equation in terms of the wave function which predicts analytically and precisely the probability of events or outcome [3]. The kinetic and potential energies are transformed into the Hamiltonian which acts upon the wave function to generate the evolution of the wave-function in position and time.

$$\hat{H}\psi(\vec{x},\vec{t}) = \hat{E}\psi(\vec{x},\vec{t}), \quad \psi(\vec{x},\vec{t}) \in \mathcal{H}$$

$\hat{H}$ and $\hat{E}$ are Hamiltonian and energy operators in a defined Hilbert Space denoted by $\mathcal{H}$. By using explicit expressions of the Hamiltonian and energy operators, we can rewrite (4) as follows

$$i\hbar \frac{\partial \psi(\vec{x},\vec{t})}{\partial \vec{t}} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(\vec{x},\vec{t})}{\partial \vec{x}^2} + V(\vec{x})\psi(\vec{x},\vec{t})$$

where the potential term has the expression of elastic potential energy

$$V(\vec{x}) = \frac{1}{2}k\vec{x}^2$$

for univariate harmonic oscillator [4]. The scalar $k$ stands for the elastic force constant. The time and position variables are denoted by overlined symbols since they will be later converted to physically dimensionless entities which will be denoted by the same symbols without overlines. The following entities with unknown scaling parameters can be defined as

$$t = \alpha \vec{t}, \quad x = \beta \vec{x}$$

which affects (5) as follows.

$$i\hbar \frac{\partial \psi}{\partial \vec{t}} = \frac{1}{2} \left( \frac{\hbar \beta^2}{m \alpha} \right) \frac{\partial^2 \psi}{\partial x^2} + \frac{1}{2} \left( \frac{k}{\hbar \alpha \beta^2} \right) x^2 \psi$$


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These two coefficients between parentheses can be set equal to any two numbers we desire since we have two arbitrary parameters, \( \alpha \) and \( \beta \). These terms encapsulated by parentheses become one to get a correspondence to the original equation’s form when \( h, m, \) and \( k \) are set equal to one.

\[
\frac{\hbar \beta^2}{m \alpha} = 1, \quad \frac{k}{\hbar \alpha \beta^2} = 1 \tag{9}
\]

The physical unitless Schrödinger equation for the univariate harmonic oscillator is found as follows.

\[
\frac{\partial \psi(x, t)}{\partial t} = \frac{-1}{2} \frac{\partial^2 \psi}{\partial x^2} + \frac{1}{2} x^2 \psi \tag{10}
\]

2 The Evolution Equations

The evolution equations are constructed using the expectation values of position and momentum respectively [1]. So, the wave function of the Schrödinger equation is implicitly used. Equation (10) can be rewritten in the following compact form in terms of the Hamiltonian operator.

\[
i \frac{\partial \psi(x, t)}{\partial t} = \hat{H}\psi(x, t), \quad \psi(x, 0) \equiv f(x) \tag{11}
\]

where we have imposed an initial form \( f(x) \) to the wavefunction \( \psi(x, t) \). The wavefunction \( \psi(x, t) \) and its initial form \( f(x) \) belong to the Hilbert space of square integrable function over the real axis.

\[
\frac{\partial \psi(x, t)}{\partial t} = -i \hat{H}\psi(x, t), \quad \psi(x, t) \in \mathcal{H} \tag{12}
\]

In the above equation if \( t \) is taken as 0, then

\[
\left( \frac{\partial \psi(x, t)}{\partial t} \right)_{t=0} = -i \hat{H}\psi(x, 0) \tag{13}
\]

can be written. If the same function is temporally differentiated, then

\[
\frac{\partial^2 \psi(x, t)}{\partial t^2} = -i \hat{H}\frac{\partial \psi(x, t)}{\partial t}, \quad \psi(x, t) \in \mathcal{H} \tag{14}
\]

is obtained and by setting \( t = 0 \)

\[
\left( \frac{\partial^2 \psi(x, t)}{\partial t^2} \right)_{t=0} = (-i \hat{H})^2 \psi(x, 0) \tag{15}
\]

can be obtained. By induction theorem:

\[
\left( \frac{\partial^k \psi(x, t)}{\partial t^k} \right)_{t=0} = (-i \hat{H})^k \psi(x, 0), \quad \psi(x, t) \in \mathcal{H} \tag{16}
\]

By using the Maclaurin Expansion [5] of the \( \psi(x, t) \):

\[
\psi(x, t) = \sum_{k=0}^{\infty} \frac{t^k}{k!} \left( \frac{\partial^k \psi(x, t)}{\partial t^k} \right)_{t=0} = \sum_{k=0}^{\infty} \frac{t^k}{k!} (-i \hat{H})^k \psi(x, 0) = e^{-i t \hat{H}} \psi(x, 0) \tag{17}
\]

Since the initial form of \( \psi(x, t) \) is \( f(x) \) we can write

\[
\psi(x, t) = e^{-i t \hat{H}} f(x), \quad f(x) \in \mathcal{H}. \tag{18}
\]

The last step of the evolution equations construction is to get differential equations to determine the expectation values. The expectation value of \( x \) is defined as follows.

\[
<x> = \langle \psi^*, x \psi \rangle = \int_V dV \psi^* x \psi = \int_V dV (e^{it \hat{H}} f x e^{-i t \hat{H}} f) \tag{19}
\]

If \( \langle x \rangle \) is temporally differentiated, then

\[
\frac{d <x>}{dt} = \int_V dV (e^{it \hat{H}} f [i \hat{H} x - x \hat{H}] e^{-i t \hat{H}} f)
\]
\[
= \int_V dV (e^{it \hat{H}} f (-i \frac{\partial}{\partial x} e^{-i t \hat{H}} f)
\]
\[
= <p> \tag{20}
\]

is obtained. The matrix representation of \( <x> \) and \( <p> \) are \( \mathbf{X} \) and \( \mathbf{P} \) respectively. Then the first evolution equation appears to be

\[
\dot{\mathbf{X}}(t) = \mathbf{P}(t) \tag{21}
\]

where \( \mathbf{X} \) and \( \mathbf{P} \) are \( n \times n \) matrices. The temporal differentiation of \( <p> \) gives

\[
\frac{d <p>}{dt} = \int_V dV (e^{it \hat{H}} f [(-i \frac{\partial}{\partial x})]
\]
\[
= \int_V dV (e^{it \hat{H}} f (-i \frac{\partial}{\partial x} V(x) e^{-i t \hat{H}} f)
\]
\[
= <f> \tag{22}
\]

If the matrix representation of \( <f> \) which can be considered an algebraic multiplication operator which multiplies it operand by \( f(x) \) is denoted by \( \mathbf{F} \) then the second evolution equation is revealed as follows

\[
\dot{\mathbf{P}}(t) = \mathbf{F}(t) \tag{23}
\]
\section{Approximated Solution}

In order to find the approximated solution for different values of \( n \), the matrix representation of \( \langle f, g \rangle \) is approximately evaluated by using fluctuationlessness theorem. We used three important definitions.

\begin{definition}
Hilbert Space [6]:
\[ \mathcal{H} \equiv \{ u_i(x) \}_{i=0}^{\infty} \]  
\[ (f, g) \equiv \int_{-\infty}^{\infty} dx f(x)g(x) \quad f(x), g(x) \in \mathcal{H} \]
\end{definition}

\begin{definition}
Integral Operator [6]:
\[ g(x) \equiv P^{(n)}g(x), \quad g(x) \in \mathcal{H}^{n} \]
\end{definition}

\[ P^{(n)} \]

\begin{definition}
\( \hat{x} \) Operator [6]:
\[ \hat{x}g(x) = xg(x), g(x) \in \mathcal{H} \]
\end{definition}

In order to project to \( \mathcal{H}^{n} \):

\[ P^{(n)} \hat{x}g(x) = P^{(n)} \hat{x} P^{(n)} g(x) = h(x) \]

\[ h_i = \sum_{j=1}^{n} (u_i, P^{(n)} \hat{x} P^{(n)} u_j) g_j \]

\[ h = X^{(n)} g \]

The matrix representation of \( \hat{x} \) is

\[ X^{(n)}_{i,j} \equiv (u_i, P^{(n)} \hat{x} P^{(n)} u_j) \]

\begin{theorem}
Fluctuationlessness Theorem [2]: In the absence of fluctuation, an algebraic multiplication–by–a–function operator’s matrix representation in any \( n \) dimensional subspace of the Hilbert space which is domain and range of the operator is same as the image of the independent variable’s matrix representation under that function within the same subspace.
\end{theorem}

\textbf{Proof:}

\[ \hat{\varphi} \approx (P^{(n)} + \left[ \hat{I} - P^{(n)} \right]) \hat{x} \left[ P^{(n)} + \left[ \hat{I} - P^{(n)} \right] \right] \]

\[ \approx P^{(n)} \hat{x} P^{(n)} \]

\[ + P^{(n)} \hat{x} \left[ \hat{I} - P^{(n)} \right] \hat{I} \left[ \hat{I} - P^{(n)} \right] \]

\[ = \hat{\varphi}_{\text{approx}} + \hat{\varphi}_{\text{fluc}} \]

This takes us to the Fluctuationless Approximation:

\[ f \approx f(\hat{\varphi}_{\text{approx}}) = f(P^{(n)} \hat{x} P^{(n)}) \Rightarrow \]

\[ P^{(n)} \approx f(X^{(n)}) \]

The evolution equations now can be converted to the following one–unknown–form:

\[ \dot{X}(t) = -X(t), \quad X(0) = A \quad \dot{X}(0) = B \]

By using the exact solution obtaining methods of ODEs

\[ X(t) = C_1 \sin(t) + C_2 \cos(t) \]

and from the initial conditions

\[ X(t) = B \sin(t) + A \cos(t) \]

can be concluded.

\section{Exact Solution}

As very well known, the eigenfunctions of the univariate harmonic oscillator has a Gauss type exponential function [4]. Hence it is better to deal with the cases where the initial form of the wave function has an exponential function whose argument is a second degree polynomial in position coordinate

\[ f(x) \equiv \psi(x, 0) = Ae^{-\gamma_1(x-x_0)^2+i\gamma_2x} \]

where \( x_0, \gamma_1 \) and \( \gamma_2 \) are assumed to be given parameters and \( A \) should be determined in such a way that the integral of the complex modulus square of the initial wavefunction over the real position values takes a specific values we impose. Since the complex modulus square of the wave function corresponds to the harmonic oscillator’s total probability of being at all points of the real axis, it must be equal to one for all time instants of the quantum motion. That is,

\[ \int_{-\infty}^{\infty} dx f^*(x)f(x) = 1 \Rightarrow A = \left( \frac{2\gamma_1}{\pi} \right)^{\frac{1}{4}} \]

The initial expectation value of \( \hat{x} \) is defined through the following equality.

\[ \langle \hat{x} \rangle_{t=0} = \int_{-\infty}^{\infty} dx f^*(x)x f(x) = x_0 \]

This result means that the expectation value of the position operator at the beginning of the evolution coincides the location of the Gauss packet represented by
$f(x)$. The initial expectation value of $\hat{p}$ is evaluated through the following equality

$$
\langle \hat{p} \rangle_{t=0} = \int_{-\infty}^{\infty} dx f^*(x) \left( -i \frac{\partial}{\partial x} \right) f(x) = \gamma_2
$$

which means that the parameter $\gamma_2$ can be replaced by the symbol $p_0$ to recall the initial momentum value. To interprete the parameter $\gamma_1$ using the initial expectation value of $\hat{x}^2$ we can use the expactation value of position square as follows.

$$
\langle \hat{x}^2 \rangle_{t=0} = \int_{-\infty}^{\infty} dx f^*(x)x^2 f(x) = \frac{A^2}{(2\gamma_1)^2} \Gamma \left( \frac{3}{2} \right) + x_0^2
$$

The initial value of the standart deviation is

$$
\langle \hat{x}^2 \rangle_{t=0} - \langle \hat{x} \rangle^2_{t=0} = \frac{1}{4\gamma_1} \Rightarrow \gamma_1 = \frac{1}{4\sigma_0}
$$

which permits to rewrite $f(x)$ in terms of three important entities, standard deviation, initial values of average position and average momentum as follows

$$
f(x) = \exp \left( -\frac{1}{4\sigma_0^2} (x - x_0)^2 + ip_0 x \right) \times \exp \left( -\frac{1}{4} \ln (2\pi\sigma_0^2) \right)
$$

This inspires us to propose the following structure for the wavefunction

$$
\psi(x, t) = \exp \left( \nu_2(t)x^2 + \nu_1(t)x + \nu_0(t) \right)
$$

where the temporally varying functions $\nu_0(t)$, $\nu_1(t)$, and $\nu_2(t)$ are undetermined yet. If we insert this structure into (10) then, second degree polynomials is found with time dependent coefficients at both sides after cancellation of the exponential functions. This implies the following ODEs whose initial conditions can be constructed using (43).

$$
\frac{id\nu_0}{dt} = \frac{1}{2} - 2\nu_2(t)^2, \nu_0(0) = -\frac{1}{4\sigma_0^2}
$$

$$
\frac{id\nu_1}{dt} = -2\nu_1(t)\nu_2(t), \nu_1(0) = \frac{x_0}{2\sigma_0^2} + ip_0
$$

$$
\frac{id\nu_2}{dt} = -\nu_2(t) - \frac{\nu_1(t)^2}{2}, \nu_0(0) = \frac{x_0^2}{4\sigma_0^2} + \ln \left( \frac{2\pi\sigma_0^2}{4} \right)
$$

Solution of these ODEs are given below

$$
\nu_0(t) = -\frac{1}{4} \left[ n(\pi) - \frac{1}{2} q(t)^2 - \frac{it}{2} \right] + \frac{i}{2}(\nu_0^2 - p_0^2) \sin(t) \cos(t) - \frac{ix_0 p_0}{2} \sin(t)
$$

$$
\nu_1(t) = q(t) + ip(t)
$$

$$
\nu_2(t) = -\frac{1}{2}
$$

where

$$
q(t) = x_0 \cos(t) + p_0 \sin(t)
$$

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

After finding the explicit value of $\psi(x, t)$, the exact value of the expectation value of $x$ at instant $t$ can be expressed as follows.

$$
\langle x \rangle = (\psi^*, x\psi) = q(t)
$$

The exact solution is therefore:

$$
\langle x \rangle = x_0 \cos(t) + p_0 \sin(t)
$$

5 Results

The matrix $A$ in the approximated solution is the matrix representation of $x_0$ in the exact solution. We have inspected how close $A$ is to $x_0$ when the value of $n$ increases.

$$
X(0)^{(n)} = A
$$

$$
A = \left[ \begin{array}{ccc} (u_1, xu_1) & \cdots & (u_1, xu_n) \\
\vdots & \ddots & \vdots \\
(u_n, xu_1) & \cdots & (u_n, xu_n) \end{array} \right]
$$

$u_i$ $(i = 1, \ldots, n)$ are the orthonormal basis functions of the Hilbert Space. They have been constructed via Cholesky Decomposition procedure [7] of MuPAD in our implementations.

To proceed to the matrix representations we define a vector $f$ is defined by using truncated linear combination structure of $\psi(x, 0) = f_1 u_1 + f_2 u_2 + \cdots + f_n u_n$ as follows.

$$
f = [f_1 f_2 \ldots f_n]
$$

Figure 1 contains the plot comparing $f^* X f$ and $x_0$. As can be noticed from that plot, the expectation value gets closer to the actual value as $n$ grows unboundedly. For the error analysis, the integral $\int_{-\infty}^{\infty} f^* f$ is used. At the infinite limit of $n$, the value of the integral is exactly one. We computed the value of the
integral for different \( n \) values and saw that it is very close to 1 when \( n \) grows up. The results are shown in Figure 2.

6 Concluding Remarks

The main goal of this work has been the testing of the applicability of the fluctuationlessness theorem on the solution of ordinary matrix differential equations of quantum dynamical systems. However the chosen potential energy function was rather simple and limited. Here we saw that the theorem can be applied for finding good approximated solutions. This encourages us to apply the theorem to more complicated functions and general cases. Our main purpose is to continue to work with solution of the systems having these kind of potential energy functions for future.

References:

[2] M. Demiralp, Fluctuation Expansion at the Horizon as a New and Efficient Tool For Integration and ODE and PDE Solving (submitted)