

A probabilistic foundation for dynamical systems: theoretical background and mathematical formulation

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Abstract In this paper we describe a probabilistic framework for describing dynamical systems. The approach is inspired by quantum dynamical expectation dynamics. Specifically, an abstract evolution operator corresponding to the Hamiltonian in quantum dynamics is constructed. The evolution of this operator defining PDE's solution is isomorphic to the functional structure of the wave function as long as its initial form permits. This operator enables us to use one of the most important probabilistic concepts, namely expectations. The expectation dynamics are governed by equations which are constructed via commutator algebra. Based on inspiration from quantum dynamics, we have used both the independent variables and the symmetric forms of their derivatives. For construction of the expectation dynamics, the algebraic independent variable operators which multiply their operands by the corresponding independent variable suffice. In our descriptions, we remain at the conceptual level in a self-consistent manner. The phenomenological implications and the tremendous potential of this approach for scientific discovery and advancement is described in the companion to this paper.

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1 Introduction

Dynamical systems are commonly described by ordinary differential equations (ODEs) where the dynamics of the system is characterized by the evolution of variables that represent position and momentum. While this representation is a tremendously useful tool in many domains, it is well known that it is insufficient in the context of the quantum dynamical descriptions which are necessary to characterize dynamics of atomic particles such as the electron, proton and others. Instead, the well known Schrödinger equation, which is a parabolic partial differential equation is used to characterize such systems. The solution of this equation is called the wave function and it does not directly define the measurable values of position or momenta. Instead, its complex modulus square defines the probability amplitude which can be used to evaluate the expectation values of operators corresponding to the observable entities like positions and momenta. The dynamical equations define the evolution of the wave function or the probability density in time. In order to find the evolutions of the expectation values, we use the inner product of the wave function with the image of the wave function under the considered operator's action. This approach allows us to construct ordinary differential equations for these expectation values. While this issue has been well studied in earlier research, we believe that a summarizing review is warranted. We devote one of the sections to this very topic.

The expectation values represented by the quantum dynamical equations have similarities to the system's classical counterpart. However, one fundamental difference is the number of unknowns. In the case of quantum dynamical equations, the number of unknowns is denumerably infinite whereas the classical equations contain as many unknown temporal functions as the system's degrees of freedom. Usually, the unknowns in the classical case are positions and momenta. Accordingly, their quantum counterparts are expectation values of the position and momenta operators. It is important to note that, due to the probabilistic nature of quantum dynamics, the expectation value of the power of an operator is not equal to the same power of the expectation value of the considered operators. This discrepancy is related to the degree of sharpness in the localization of the wave function in space. We refer to this discrepancy as “mathematical fluctuations”. They are the essential reasons for the infinite number of unknowns in the quantum expectation value dynamics. We also devote one of the subsequent sections to the discussion of this topic.

This paper is fundamentally based on the similarities and discrepancies between classical and quantum expectation dynamics. The details will be presented after the abovementioned sections. The potential phenomenological implications of this work will be described in a separate but companion paper to the this one. This companion also contains discussion specifically about dynamical systems based causal modeling frameworks as they are currently used in neuroscience and human functional neuroimaging. While we are thrilled about the cross disciplinary pollination of ideas and potential for discovery, we leave such discussions solely to the companion paper.

The paper is organized as follows. The Sects. 2 and 3 summarize the essential features of equations characterizing classical and quantum expectation dynamics. The Sect. 4 introduces previous research on the concept of mathematical fluctuations. The Sect. 5 focuses on the basis operators and commutators while the Sect. 6 expands upon approaches for finding the appropriate Hamiltonian structures. Building on this structure, the Sect. 7 proceeds to formulate the generalized expectation dynamics. In this section, approaches for constructing a simple and efficient Hamiltonian are described. In the Sect. 8, the solution of the evolution equation based on the abovementioned Hamiltonian is formulated. The Sect. 9 summarizes the steps for constructing the probabilistic framework for dynamical systems. This section which is a culmination of all the subsequent sections leads up to an extremely important linearization procedure. The Sect. 10 finalizes the paper with concluding remarks. This paper is designed to be comprehensive in a canonical fashion, therefore we focus on formulating an expansive mathematical framework. In future research, numerical implementations that are relevant to specific fields of science will be described.

2 Dynamical systems

A dynamical system's state is mathematically defined by a set of real numbers. These can also be called vectors since these values can represent a point in an appropriate Cartesian space called either "state space" or "phase space", for a specified time instant denoted by t . Hence the state vector which can be denoted by $\mathbf{x}(t)$ is composed of temporal elements denoted by $x_1(t), \dots, x_n(t)$. The time variable generally takes nonnegative real values although it is sometimes more efficient to consider all real values. While it is possible to use integer domains for t as commonly used in cascaded systems, in this paper we will focus on the continuous cases. The dynamical system is essentially defined by providing a rule for time evolution of its state. This rule is generally differential, which means that the differential change in the state vector is given for any time instant t . This can be done by defining an ordinary differential equation with appropriate initial conditions to get uniqueness. Thus, the determination of the considered dynamical system's evolution requires the solution of the ODE initial value problem mentioned above. In other words, the evolution necessitates integration which may not be accomplished analytically for all possible cases. Therefore the governing equations for a dynamical system [1,2] can be written as follows

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t)), \quad t \in [0, \infty), \quad \mathbf{x}(0) = \mathbf{a} \quad (1)$$

$$\mathbf{x}(t) \equiv [x_1(t) \dots x_n(t)]^T \quad (2)$$

where dot stands for the temporal differentiation and the set of ODE is assumed to be autonomous without any loss of generality since nonautonomous structure can be removed by adding a new temporal function equal to just t . The initial value vector, \mathbf{a} and \mathbf{f} 's functional structure are given.

The solution of the initial value problem given through (1) may not be analytically possible depending on the functional dependence of $\mathbf{f}(\mathbf{x})$ on the state vector. While the linear or affine structures allow us to get analytical solutions, the other structures

which are nonlinear may lead to analytic solutions only in a limited number of cases. While this is an important issue, it is a technical one, therefore we do not elaborate on its implications here.

Beyond the feasibility of analytic solution, the other important issue is the causality. This means that a so-called trajectory or orbit, completely defined by the temporal variation of the state vector, never bifurcates. This property can be provided only by restricting the functional structure of \mathbf{f} appropriately. Otherwise the system may have more than one state at some time instances for a given single initialization. This issue is also kept outside the content of the paper.

3 Fluctuation free quantum expectation dynamics

Consider a quantum system [3,4] whose Hamiltonian, which is a second order linear partial differential operator in spatial coordinate(s), is denoted by $\widehat{H}(t)$. Its dynamics is governed by the following equation

$$i\hbar \frac{\partial \psi}{\partial t} = \widehat{H}(t)\psi \quad (3)$$

where \hbar stands for the reduced Planck constant while ψ denotes the wave function depending on both time (t) and position (x). The Hamiltonian is composed of terms including the position and momentum operator(s) in addition to certain temporally varying entities. In this formulation, we have shown only the temporal dependence because of its importance in the dynamical characterization.

The wave function is a complex valued entity and its complex modulus square is the probability density of the quantum system under consideration. The wave function can be considered as lying in an Hilbert space where the inner product of two functions is defined as the multidimensional integral of the product of one function with the other's complex conjugate. This inner product induces a norm definition which corresponds to the integral of the complex modulus square of the target function to norm. The integration domain is a matter of modelling however appropriate boundary conditions must be imposed to provide self-adjointness or in other words Hermiticity. Regarding these facts, one can say that the norm of the wave function can be taken 1 for all time instances as can be proven from the equation in (3) and its complex conjugate.

The norm preserving property of the wave function enables us to give a probabilistic nature to it. This also facilitates the expected value (or expectation) definition of an operator. The expectation of an operator, say \widehat{O} , is defined as the inner product of the wave function with its image under the considered operator and therefore can be explicitly given by the following identity

$$o(t) \equiv \langle \widehat{O} \rangle(t) \equiv (\psi(t), \widehat{O}\psi(t)) \quad (4)$$

where we have not explicitly shown the dependence of the wave function on spatial variables since they are internal agents of the inner product as being the dummy integration variables. The expectation should depend on time due to the temporal nature of the wave function and it is explicitly shown after the left and right angle symbols.

If we now temporally differentiate both sides of (4), after assuming the time independence of the operator \widehat{O} , we can write

$$\begin{aligned}\dot{o}(t) &= \left(\frac{\partial \psi(t)}{\partial t}, \widehat{O} \psi(t) \right) + \left(\psi(t), \widehat{O} \frac{\partial \psi(t)}{\partial t} \right) \\ &= \left(-\frac{i}{\hbar} \widehat{H}(t) \psi(t), \widehat{O} \psi(t) \right) + \left(\psi(t), \widehat{O} \left(-\frac{i}{\hbar} \widehat{H}(t) \right) \psi(t) \right) \\ &= \left(\psi(t), \left\{ \frac{i}{\hbar} [\widehat{H}(t) \widehat{O} - \widehat{O} \widehat{H}(t)] \right\} \psi(t) \right)\end{aligned}\quad (5)$$

where we have used (3) and the Hermiticity of the Hamiltonian operator.

In most of the quantum models, the Hamiltonian of the system is time invariant as long as it is isolated from its environment. In other words, time dependence is assumed to be coming from the external influences which generally appear in the potential or potential-like (for example vector field reflecting terms under the strong magnetic fields) parts of the Hamiltonian. This urges us to write the following structure for the Hamiltonian with minimal loss of generality

$$\widehat{H}(t) \equiv \widehat{H}_{\text{iso}} + \sum_{j=1}^m h_j(t) \widehat{H}_j \quad (6)$$

where $h_j(t)$ s are given real valued temporal functions while the \widehat{H}_j s are Hermitian operators depending on the position and momentum operator(s) whereas \widehat{H}_{iso} is the Hamiltonian of the system when it is isolated from its environment. We can now use (6) in (5) to get

$$\begin{aligned}\dot{o}(t) &= \left(\psi(t), \left\{ \frac{i}{\hbar} [\widehat{H}_{\text{iso}} \widehat{O} - \widehat{O} \widehat{H}_{\text{iso}}] \right\} \psi(t) \right) \\ &\quad + \sum_{j=1}^m h_j(t) \left(\psi(t), \left\{ \frac{i}{\hbar} [\widehat{H}_j \widehat{O} - \widehat{O} \widehat{H}_j] \right\} \psi(t) \right)\end{aligned}\quad (7)$$

which contains $m + 1$ new time invariant operators at its right hand side inside the pairs of curly braces. This means that the temporal derivative of a given operator's expectation is a linear combination of the expectations for the commutators (or Poisson brackets in quantum mechanical terminology) of the system's Hamiltonian with the spatial components of the same Hamiltonian. Since the latter expectations may not also be explicitly known unless some specific conditions are fulfilled, we need to derive differential equations for the expectations of these new operators by tracing the route we have followed to obtain (7). This procedure results in the birth of new operators and as we proceed the expectations populate towards infinity unless some closedness conditions amongst these operators exist. We do not get into the technical details here. What we can say as a conclusion is that an infinite set of ODEs governs the dynamics of the expectations. The key agents in the construction of these equations are the choice of the operator to start the procedure and the Hamiltonian (therefore the

model) structure. One starting choice may end up at a finite set of operators while the other may require infinite number of operators. This is a commutator algebraic issue and we will not get into its details.

Before going further, we need to focus a little bit on the structures of the operators \widehat{H}_{iso} and \widehat{H}_j s. As we mentioned above, they are generally depending on the position and momentum operators. However their dependence on these operators plays important roles for the structuring of the expectation dynamical equations. To show this, we may consider the case where the system does not interact with its environment. In other words all \widehat{H}_j s vanish. As another simplicity we may consider the system as a one dimensional model whose spatial variable is denoted by x . In this case the position (\widehat{x}) and momentum (\widehat{p}) operators are defined in terms of the spatial variables for an arbitrary function $f(x, t)$ differentiable at least once in t

$$\widehat{x}f(x, t) \equiv xf(x, t), \quad \widehat{p}f(x, t) \equiv -i\hbar \frac{\partial f(x, t)}{\partial x} \tag{8}$$

where t , time, takes nonnegative values while the spatial variable is assumed to get real values. The operator \widehat{x} is an algebraic multiplication operator which multiples its operand by the independent variable while the momentum operator \widehat{p} spatially differentiates its operand and then multiplies the result by $-i\hbar$. Both of these operators have continuous spectra and therefore have distributional or generalized function type eigenfunctions. Our system is chosen as a single particle under the influence of a potential function denoted by $V(x)$ for sufficient simplicity and generality. We can write

$$\widehat{H} \equiv \widehat{H}_{iso} \equiv -\frac{1}{2\mu} \widehat{p}^2 + V(\widehat{x}) \tag{9}$$

where μ stands for the mass parameter of the particle under consideration. It is not hard to see that the following commutation rule holds

$$\widehat{H}\widehat{x} - \widehat{x}\widehat{H} = -i\frac{\hbar}{\mu} \widehat{p} \tag{10}$$

which urges us to take \widehat{O} as \widehat{x} and to obtain

$$\dot{o}(t) \equiv \dot{\xi}(t) = \frac{1}{\mu} \pi(t), \quad \pi(t) \equiv \langle \widehat{p} \rangle (t), \quad \xi(t) \equiv \langle \widehat{x} \rangle (t). \tag{11}$$

If we would take \widehat{O} as \widehat{p} then we would get

$$\dot{o}(t) \equiv \dot{\pi}(t) = -\langle V'(\widehat{x}) \rangle \tag{12}$$

Equations (11) and (12) becomes sufficient to solve both $\xi(t)$ and $\pi(t)$ without leaving any uncertainty when the potential function $V(x)$ is a polynomial with a degree less than three since its expectation becomes a first degree polynomial in $\xi(t)$. Otherwise these two equations are not sufficient to get a solution since the expectation of the

operator $V'(\hat{x})$ becomes no longer expressible in terms of only the operator \hat{x} . In order to compensate for this one needs to construct more ODEs and this procedure may never end.

The at-most-second-degree polynomial structure in the potential function $V(x)$ is a great limitation to get equations to be simultaneously solved for $\xi(t)$ and $\pi(t)$ and is provided by only harmonic oscillator or free particle. In this case the following equality remains valid

$$\langle V'(\hat{x}) \rangle = V'(\langle \hat{x} \rangle) \quad (13)$$

Even though its validity breaks down for other V functions we may nevertheless have an asymptotic relation as long as the wave function is sufficiently narrowly spreaded (if it becomes an infinite jump like Dirac's delta function then relation becomes exact).

$$\lim_{\psi \rightarrow \delta_D} \langle V'(\hat{x}) \rangle = V'(\langle \hat{x} \rangle) \implies \langle V'(\hat{x}) \rangle \approx V'(\langle \hat{x} \rangle) \quad (14)$$

All fluctuations in the operator expectations vanish when the wave function becomes similar to the Dirac delta function. In this case the quantum mechanics approaches classical mechanics. Therefore by assuming that the wave function is sufficiently sharply localized, we can approximate the expectation of $V'(\hat{x})$ by $V'(\langle \hat{x} \rangle)$. This approximation corresponds to the application of the Fluctuationless Theorem [5–12] to the one dimensional matrix representation case and the error diminishes as the first basis function there tends to become Dirac delta function.

Now we can get the following ODEs for abovementioned $\xi(t)$ and $\pi(t)$ functions which are the expectations of the position and momentum operators respectively

$$\dot{\xi}(t) = \frac{1}{\mu} \pi(t), \quad \dot{\pi}(t) = -V'(\xi(t)) \quad (15)$$

which are two ODEs on two unknowns. These are obtained in fact by assuming all of the expectations of any type product of the position and momentum operators is equal to the same product of not the operators but their expectations. These entities deviate from each others and the deviations are defined as fluctuations. Hence we assume all fluctuations are vanishing. Hence we call these equations “Fluctuation Free Expectation Dynamics” of the considered system.

If the fluctuations are not ignored then we need to define some other operators and construct ODEs for their expectations. This procedure results in an infinite set of linear ODEs unless the Hamiltonian has a very specific structure. This issue and the relevant details of Mathematical Fluctuation Theory will be focused on in the coming sections.

4 Mathematical fluctuation theory

Let us consider an Hilbert space (\mathcal{H}) of univariate functions which are analytic in a certain region of the complex plane of their arguments such that the analyticity region

involves the integration interval of the inner product for that space. If we take the basis set Υ spanning \mathcal{H} and its N -term finite restriction Υ_N defined as follows

$$\Upsilon \equiv \{v_j(x)\}_{j=1}^\infty, \quad \Upsilon_N \equiv \{v_j(x)\}_{j=1}^N \tag{16}$$

then we can use the symbol \mathcal{H}_N to denote the subspace spanned by Υ_N . Any linear operator from \mathcal{H} to \mathcal{H} has a unique restriction over \mathcal{H}_N (it maps from \mathcal{H}_N to \mathcal{H}_N). Now we can consider the mapping from linear operators (from \mathcal{H} to \mathcal{H}) to matrix representations over the restricted basis set $v_1(x), \dots, v_N(x)$ and denote it by $\mathbf{M}_N(\hat{O})$ for the mapping from the operator \hat{O} to its restricted matrix representation. We can write the following equality for any two different linear operators denoted by \hat{O}_1 and \hat{O}_2 mapping from \mathcal{H} to \mathcal{H}

$$\begin{aligned} \mathbf{M}_N(\hat{O}_1 \hat{O}_2) &\equiv \mathbf{M}_N(\hat{O}_1 \hat{P}^{(N)} \hat{O}_2) + \mathbf{M}_N(\hat{O}_1 [\hat{I} - \hat{P}^{(N)}] \hat{O}_2) \\ &\equiv \mathbf{M}_N(\hat{O}_1) \mathbf{M}_N(\hat{O}_2) + \mathbf{M}_N(\hat{O}_1 [\hat{I} - \hat{P}^{(N)}] \hat{O}_2) \end{aligned} \tag{17}$$

where the operator $\hat{P}^{(N)}$ projects to the subspace spanned by the restricted basis set Υ_N . As can be immediately noticed, the operator $[\hat{I} - \hat{P}^{(N)}]$ approaches the zero operator as N goes to infinity. The complement of the space spanned by the finite set $\{v_1(x), \dots, v_N(x)\}$ to the entire Hilbert space, \mathcal{H}_N^\perp is spanned by the functions which become more oscillatory as N grows. Therefore any function in this complementary space fluctuates more rapidly as N increases. Hence we call the operator $[\hat{I} - \hat{P}^{(N)}]$ ‘‘Fluctuation Operator’’, and parallel to this, we call any expectation containing operators where the fluctuation operator appears once or more than once ‘‘Fluctuation Term’’. Hence the last term in (17) stands for a fluctuation term. If we ignore all fluctuation terms in a formula then we call what we get ‘‘Fluctuationlessness Approximation’’ or ‘‘Fluctuation Free Version’’ of the formula. Thus, the fluctuation free version of (17) can be written as follows

$$\mathbf{M}_N(\hat{O}_1 \hat{O}_2) \approx \mathbf{M}_N(\hat{O}_1) \mathbf{M}_N(\hat{O}_2) \tag{18}$$

The consecutive utilization of this approximation allows us to write

$$\mathbf{M}_N(\hat{x}^m) \approx \mathbf{M}_N(\mathbf{x})^m \equiv \mathbf{X}_N^m, \quad m = 1, 2, \dots \tag{19}$$

where \mathbf{X}_N stands for the matrix representation of the independent variable as noticed. This implies

$$\mathbf{M}_N(f(\hat{x})) \approx f(\mathbf{M}_N(\hat{x})) = f(\mathbf{X}_N) \tag{20}$$

where the function f is assumed to be analytic in a complex region of its argument, including the origin. Here we have dealt with the matrix representation of the algebraic function multiplication operator, \hat{f} , which multiplies its operand by the function $f(x)$. We called the matrix \mathbf{X}_N ‘‘Universal Matrix’’ since it is the matrix representation of

the independent variable and therefore does not depend on any functional structure in contrast to function multiplication operator.

The formula in (20) is the mathematical expression of the “Fluctuationlessness Theorem”[6] conjectured and proven by the first author. It states that the matrix representation of a function multiplication operator is equal to the image of the universal matrix over the subspace spanned by the first N number of basis functions for the entire Hilbert space when all fluctuations are ignored. The theorem is valid as long as some level of analyticity exist in the function under consideration. The multivariate counterpart of this theorem is also valid as it is shown by the first author.

We find this summary material sufficient for our purposes here.

5 Basis operators and commutators

The Taylor expansion of a univariate function is an infinite linear combination of powers like $(x - a)^k$ where k is a nonnegative integer while x and a stand for the independent variable and the expansion point. Hence these powers can be considered as the basis set of the function space under consideration. Since we deal with the operators in the quantum expectation dynamics, it is better to consider some basis operators. Let us go back to the section of fluctuation free quantum expectation dynamics. There we had assumed that the system’s Hamiltonian can be represented in terms of continuous functions of the position and momentum operators which are corresponding somehow to the abovementioned independent variable. This and the brief discussion above bring the idea of using the products of powers of these operators as the basis operators to represent an arbitrary operator assumed to be continuously depending on these operators. We need to start with the zeroth powers first as we do in the case of Taylor series. The only operator which contains the zeroth powers of the position and momentum operators is the unit operator, \widehat{I} . This corresponds to the constant term of the Taylor series where the basis function is the unit constant function.

Now, to proceed, we can deal with the powers of the operators $(\widehat{x} - a\widehat{I})$ and $(\widehat{p} - a\widehat{I})$. Choosing a nonzero takes us to the Taylor series while the zero a value corresponds to Maclaurin series. We will prefer to take $a = 0$ for simplicity here. Thus, the first degree linearly independent basis operators can be \widehat{x} and \widehat{p} . We have now three basis operators and obviously the commutators of the \widehat{x} and \widehat{p} with \widehat{I} vanish while the following equality can be obtained to show the mutual non commutativity of \widehat{x} and \widehat{p}

$$\widehat{x}\widehat{p} - \widehat{p}\widehat{x} = i\hbar\widehat{I} \quad (21)$$

To construct the second degree basis operators we have four chances: \widehat{x}^2 , $\widehat{x}\widehat{p}$, $\widehat{p}\widehat{x}$ and \widehat{p}^2 . However, the second and third operators are not Hermitian despite the Hermiticity of the position and momentum operators over the space of functions vanishing at the ends of the interval (generally we deal with to use entire real axis for the domain of x unless some geometrical enforcements do not show up). Hence, instead of them, their symmetrized linear combinations can be considered as the basis operators. There are two possibilities to this end, $(\widehat{x}\widehat{p} + \widehat{p}\widehat{x})$ and $i(\widehat{x}\widehat{p} - \widehat{p}\widehat{x})$. Only the first possibility can be used since the second one is proportional to the unit operator and therefore

its degree is zero not two as appeared. All these mean that the possible Hermitian second degree basis operators can be chosen as \widehat{x}^2 , $\frac{1}{2}(\widehat{x}\widehat{p} + \widehat{p}\widehat{x})$ and \widehat{p}^2 . These are the symmetric and nonreducible (which can not be represented as a linear combination of the lower degree terms only) second degree operators.

The above analysis can be generalized to higher degrees without any remarkable difficulty. This procedure results in the following basis operators which are Hermitian and irreducible compositions of binary products

$$\widehat{o}_{n,j}^{(bas)} \equiv \frac{1}{2} \left(\widehat{x}^{j-1} \widehat{p}^{n+1-j} + \widehat{p}^{n+1-j} \widehat{x}^{j-1} \right), \quad n = 0, 1, \dots \quad j = 1, 2, \dots, n + 1 \tag{22}$$

One can of course ask what happens to products of more than two factors. It is not hard to show that they can be expressed as linear combinations of binary products whose degree are equal to or less than their own degrees. We call the operators in (22) ‘‘Basis Operators’’. The commutator of any two basis operators can be expressed in terms of the same basis operators. In other words

$$\widehat{o}_{n_1,j_1}^{(bas)} \widehat{o}_{n_2,j_2}^{(bas)} - \widehat{o}_{n_2,j_2}^{(bas)} \widehat{o}_{n_1,j_1}^{(bas)} = \sum_{n_3=0}^{\infty} \sum_{j_3=1}^{n_3+1} c_{n_1,j_1;n_2,j_2;n_3,j_3} \widehat{o}_{n_3,j_3}^{(bas)} \tag{23}$$

where c s are the elements of an infinite three way array (infinite in its each way, we consider a single direction ordering over each couple of (n, j) s). Although the word ‘‘tensor’’ is widely used for these type arrays we do not prefer its utilization since ‘‘tensor’’ in continuum mechanics have some physical features which need not to be existing in multilinear arrays. We do not intend to get into further details at this moment even though the elements of \mathbf{c} can be uniquely determined through a commutator algebraic procedure.

6 Mathematical extensions to Hamiltonian

The previously mentioned Hamiltonian operator $\widehat{H}(t)$ has some restrictive properties. One of them is the symmetry or Hermiticity and provides the real valuedness of the Hamiltonian expectation which is desired in quantum mechanics due to its relation to the total energy of the system. We do not intend to remove this restriction since our purpose is to deal with real valued items for the moment. The second property is a second degree polynomial structure in momentum. This comes from the physical nature of the quantum mechanics where the total energy of an isolated system is conserved during its evolution. This physical constraint can be removed since our purpose is not to construct a quantum dynamics but probabilistic foundation where there is no apparent need for a rule similar to energy conservation. On the other hand, there are some other probabilistic evolutionary partial differential equations like Louville equations where the order in momentum is one. Our purpose here is to get the mathematical structure as general as we can.

The other restriction we have aforementioned is the continuity of the Hamiltonian in momentum and position. The position dependence is generally controlled by potential or potential like structures and there may be some potential cases where discontinuity with respect to position may appear. However, even those cases can be approximated by some structures continuous in position. The removal of the second degree polynomiality in momentum may bring some unexpected discontinuities in momentum. Even in those cases asymptotically discontinuous continuities can handle the situation. Therefore we can propose the following structure for the system Hamiltonian operator

$$\widehat{H}(t) = \sum_{n=0}^{\infty} \sum_{j=1}^{n+1} H_{n,j}(t) \widehat{o}_{n,j}^{(\text{bas})}, \quad n = 0, 1, \dots \quad j = 1, 2, \dots, n+1 \quad (24)$$

where the temporally varying entities, $H_{n,j}(t)$ s are given real functions. This Hamiltonian may not correspond to any physically existing system. It's a hypothetical structure or in other words it is a mathematical extension to quantum dynamical Hamiltonian. Since this structure is an infinite linear combination in basis operators it is the most general dynamically changeable Hamiltonian structure in the space of Hermitian linear operators derived from position and momentum operators.

The above definition in (24) enables us to write

$$\begin{aligned} \widehat{H}(t) \widehat{o}_{n_1, j_1}^{(\text{bas})} - \widehat{o}_{n_1, j_1}^{(\text{bas})} \widehat{H}(t) &= \sum_{n_2=0}^{\infty} \sum_{j_2=1}^{n_2+1} H_{n_2, j_2}(t) \left(\widehat{o}_{n_2, j_2}^{(\text{bas})} \widehat{o}_{n_1, j_1}^{(\text{bas})} - \widehat{o}_{n_1, j_1}^{(\text{bas})} \widehat{o}_{n_2, j_2}^{(\text{bas})} \right) \\ &= \sum_{n_2=0}^{\infty} \sum_{j_2=1}^{n_2+1} \sum_{n_3=0}^{\infty} \sum_{j_3=1}^{n_3+1} H_{n_2, j_2}(t) c_{n_1, j_1; n_2, j_2; n_3, j_3} \widehat{o}_{n_3, j_3}^{(\text{bas})} \\ &= \sum_{n_2=0}^{\infty} \sum_{j_2=1}^{n_2+1} C_{n_1, j_1, n_2, j_2}(t) \widehat{o}_{n_2, j_2}^{(\text{bas})} \\ & \quad n_1 = 0, 1, \dots \quad j_1 = 1, 2, \dots, n_1 + 1 \end{aligned} \quad (25)$$

where we have used (23) and the entities defined as

$$\begin{aligned} C_{n_1, j_1, n_2, j_2}(t) &= \sum_{n_3=0}^{\infty} \sum_{j_3=1}^{n_3+1} H_{n_3, j_3}(t) c_{n_1, j_1; n_3, j_3; n_2, j_2} \\ n_1, n_2 = 0, 1, \dots \quad j_1 = 1, 2, \dots, n_1 + 1 \quad j_2 = 1, 2, \dots, n_2 + 1. \end{aligned} \quad (26)$$

The four index array C_{n_1, j_1, n_2, j_2} can be converted to an infinite matrix by reordering the indices n_1, j_1 and n_2, j_2 separately in single directions. We may call it "Folded Matrix" or shortly "Folmat". Its unfolded structure in matrix format will be denoted by $\mathbf{C}(t)$ from now on. We can now define

$$\widehat{\mathbf{o}}^{(\text{bas})} \equiv \left[o_{0,1}^{(\text{bas})} \quad \dots \quad o_{n,j}^{(\text{bas})} \quad \dots \right]^T \quad (27)$$

which permits us to arrive at the following very important result.

$$\widehat{H}(t)\widehat{\mathbf{o}}^{(\text{bas})} - \widehat{\mathbf{o}}^{(\text{bas})}\widehat{H}(t) = \mathbf{C}(t)\widehat{\mathbf{o}}^{(\text{bas})} \tag{28}$$

We will call $\mathbf{C}(t)$ “The Commutation with the Hamiltonian Matrix” for basis operator set.

7 Generalized expectation dynamics

As can be noticed easily we can write

$$\frac{d\langle \mathbf{o}^{(\text{bas})} \rangle(t)}{dt} = \frac{i}{\hbar} \left(\widehat{H}(t)\widehat{\mathbf{o}}^{(\text{bas})} - \widehat{\mathbf{o}}^{(\text{bas})}\widehat{H}(t) \right) (t) = \frac{i}{\hbar} \mathbf{C}(t) \langle \widehat{\mathbf{o}}^{(\text{bas})} \rangle (t) \tag{29}$$

If we define

$$\mathbf{o}^{(\text{bas,exp})}(t) \equiv \langle \mathbf{o}^{(\text{bas})} \rangle (t) \tag{30}$$

then we can rewrite (29) as follows

$$\dot{\mathbf{o}}^{(\text{bas,exp})}(t) = \frac{i}{\hbar} \mathbf{C}(t)\widehat{\mathbf{o}}^{(\text{bas,exp})}(t) \tag{31}$$

which is an infinite set of linear ODEs with a variant coefficient matrix.

The linearity of the infinite ODE set comes from the fact that the infinite matrix $\mathbf{C}(t)$ does not depend on expectations. However it depends on Hamiltonian and to reveal its explicit expressions is not an easy task. Nevertheless the downward determination of its rows starts with a trivially easy step and gradually increases in complication. For this reason we do not attempt to find all rows at this moment. Instead we are going to try to determine the first two rows. Let us start with the first row. We can write the following equation from (26)

$$C_{0,1,n_2,j_2}(t) = \sum_{n_3=0}^{\infty} \sum_{j_3=1}^{n_3+1} H_{n_3,j_3}(t) c_{0,1;n_3,j_3;n_2,j_2} \tag{32}$$

$n_2 = 0, 1, \dots \quad j_2 = 1, 2, \dots, n_2 + 1.$

which urges us to go back to (23) and write

$$\widehat{o}_{0,1}^{(\text{bas})}\widehat{o}_{n_2,j_2}^{(\text{bas})} - \widehat{o}_{n_2,j_2}^{(\text{bas})}\widehat{o}_{0,1}^{(\text{bas})} = \sum_{n_3=0}^{\infty} \sum_{j_3=1}^{n_3+1} c_{0,1;n_2,j_2;n_3,j_3} \widehat{o}_{n_3,j_3}^{(\text{bas})} \tag{33}$$

where the left hand side always vanishes for all (n_2, j_2) couples since $\widehat{o}_{0,1}^{(\text{bas})}$ is unit operator. This implies $c_{0,1;n_2,j_2;n_3,j_3} = 0$ since it is the coefficient in an infinite linear

combination of linearly independent (basis) functions. So we get $C_{0,1,n_2,j_2}(t) \equiv 0$ and therefore

$$\mathbf{e}_1^T \mathbf{C} = \mathbf{0}^T \quad (34)$$

where \mathbf{e}_j^T stands for the Cartesian unit vector whose nonzero element takes the value of 1 and is located in the j th position. This result, which reveals the fact that first row vanishes, leads us to the following ODE

$$o_{0,1}^{(\text{bas,exp})}(t) = 0, \quad o_{0,1}^{(\text{bas,exp})}(0) = 1 \quad (35)$$

where the imposed initial condition is due to the normalized nature of the wave function. Hence we get $o_{0,1}^{(\text{bas,exp})}(t) = 1$ which is an expected result.

We can start with the following identity for determining the second row of $\mathbf{C}(t)$

$$\begin{aligned} \widehat{x}\widehat{p}^{n+1-j} &\equiv \widehat{p}^{n+1-j}\widehat{x} + i(n+1-j)\hbar\widehat{p}^{n-j}, \\ n = 0, 1, \dots; \quad j &= 1, 2, \dots, n+1 \end{aligned} \quad (36)$$

whose validity can be shown by proving the identity of the actions of its both sides on an arbitrary sufficiently differentiable function. This leads us to get the following result after some intermediate operator algebraic manipulations

$$\widehat{x}\widehat{o}_{n,j}^{(\text{bas})} - \widehat{o}_{n,j}^{(\text{bas})}\widehat{x} = i(n+1-j)\hbar\widehat{o}_{n-1,j}^{(\text{bas})}, \quad n = 0, 1, \dots; \quad j = 1, 2, \dots, n+1 \quad (37)$$

whose comparison with the form of (23) when $n_1 = 1$ and $j_1 = 2$ reveals the following equality

$$c_{1,2;n_2,j_2;n_3,j_3} = i(n_3 + 2 - j_3)\hbar\delta_{n_3,n_2-1}\delta_{j_3,j_2} \quad (38)$$

which enables us to obtain

$$\begin{aligned} C_{1,2,n_2,j_2} &= i(n_2 + 2 - j_2)\hbar H_{n_2+1,j_2}(t), \\ n_2 = 0, 1, \dots; \quad j_2 &= 1, 2, \dots, N_2 + 1 \end{aligned} \quad (39)$$

by using (26). This gives all second row elements of the matrix $\mathbf{C}(t)$. Therefore the second ODE of the expectation dynamics can be written as follows

$$\begin{aligned} \dot{o}_{1,2}^{(\text{bas,exp})}(t) &= \sum_{n=0}^{\infty} \sum_{j=1}^{n+1} \frac{i}{\hbar} C_{1,2,n,j} o_{n,j}^{(\text{bas,exp})}(t) \\ &= - \sum_{n=0}^{\infty} \sum_{j=1}^{n+1} (n+2-j) H_{n+1,j}(t) o_{n,j}^{(\text{bas,exp})}(t) \end{aligned} \quad (40)$$

If the momentum operator does not show up anywhere at the right hand side then only the expectations of the powers of the position operator appear in the ODE. Then the utilization of the fluctuation free representations of these terms provide the dependence of right hand side only on the expectation $o_{1,2}^{(bas,exp)}(t)$. Otherwise the momentum operator's expectation unavoidably show up. This means the connection to at least a third and remaining set of expectation equations, which is completely undesirable for our purpose here since we want to get a single existing target ODE which will be obtained via fluctuation free representation. Thus we impose the following structure

$$H_{n,j}(t) = \chi_n(t)\delta_{j,n}, \quad n = 1, 2, \dots \tag{41}$$

whose employment in (24) shows that the Hamiltonian must have the following form

$$\widehat{H}(t) = a_0(t)\widehat{I} + \frac{1}{2} \{a_1(\widehat{x}, t)\widehat{p} + \widehat{p}a_1(\widehat{x}, t)\} \tag{42}$$

where $a_0(t)$ can be taken identically zero since it never enters the expectation because it contains the coefficients of the unit operator vanishing in commutation operations. This formula produces

$$\frac{i}{\hbar} [\widehat{H}(t)\widehat{x} - \widehat{x}\widehat{H}(t)] = a_1(\widehat{x}, t) \tag{43}$$

and therefore

$$\dot{\xi}(t) \equiv \langle \dot{\widehat{x}} \rangle(t) = \langle a_1(\widehat{x}, t) \rangle \approx a_1(\langle \widehat{x} \rangle, t) = a_1(\xi(t), t) \tag{44}$$

where we have used the fluctuation free representation of the right hand side. This means that an ODE given by the rightmost equation of (44) has a probabilistic foundation if the Hamiltonian's a_1 function matches the right hand side of this ODE when the position operator is replaced by $\xi(t)$.

Thus we have shown that a Hamiltonian can be constructed for any single ODE such that the expectation of the independent variable (position) over its wave function satisfies that ODE at the fluctuation free expectations limit.

8 Wave equation for probabilistic foundation

The discussions of the previous section urge us to rewrite the probabilistic foundation Hamiltonian and Wave Equation as follows

$$\widehat{H}(t) = \frac{1}{2} \{a(\widehat{x}, t)\widehat{p} + \widehat{p}a(\widehat{x}, t)\} \tag{45}$$

$$\begin{aligned} \frac{\partial \psi(x, t)}{\partial t} &= -\frac{1}{2} \left\{ a(x, t) \frac{\partial}{\partial x} - \frac{\partial}{\partial x} a(x, t) \right\} \psi(x, t) \\ &= -a(x, t) \frac{\partial \psi(x, t)}{\partial x} - \frac{1}{2} \frac{\partial a(x, t)}{\partial x} \psi(x, t) \end{aligned} \tag{46}$$

In the case where a does not depend on t we can write

$$y \equiv \int_0^x d\bar{x} \frac{1}{a(\bar{x})}, \quad \psi(x, t) = \frac{1}{\sqrt{a(x)}} \bar{\psi}(y, t) \quad (47)$$

which leads us to get

$$\frac{\partial \bar{\psi}(y, t)}{\partial t} = -\frac{\partial \bar{\psi}(y, t)}{\partial y} \quad (48)$$

whose solution is $f(y - t)$. The shape of f can be determined by using the initial form of the changed wave function, $\bar{\psi}_0(y)$ and the solution is obtained as

$$\bar{\psi}(y, t) = \bar{\psi}_0(y - t) \quad (49)$$

This is a wave structure. However it may not be just a simple translational wave unless a becomes a constant function. It is translational with respect to y but it may have quite complicated nature with respect to x depending on a . We do not intend to go beyond this level information.

Evidently, the initial form gains a lot of importance to give probabilistic nature to the wave function. We may seek some general universal features for these entities. Then their structures can be chosen and parametrized accordingly.

Since the momentum operator does not show up in the evolutionary ODE of (44), it becomes a matter of curiosity to get the evolutionary equation for its expectation. For this purpose we can use the abovementioned Hamiltonian's commutator with the momentum operator and get the desired ODE by taking expectation. This gives

$$\dot{\pi}(t) \equiv \langle \hat{p} \rangle = -\langle a_x(x, t) \hat{p} \rangle \approx -a_{\xi}(\xi(t), t) \pi(t) \quad (50)$$

where we have used the fluctuation free representation at the rightmost term and the subscript of a stands for the partial differentiation with respect to the variable symbolized by that subscript. The function $\xi(t)$ satisfies (44) after removing the index of a_1 there. The differentiation of both sides in (44) and (50) permits us to get a relation between π and its first derivative and ξ and its second derivative. Thus we can understand which kind of entity the momentum expectation is. The impression from the expectation dynamical equations of quantum mechanics the operator $a(\hat{x}, t)$ seems to play the role of the momentum in contrast to the operator \hat{p} when it has no time dependence. Even in the case of time dependence it seems to be more attractive for the utilization towards this end. Since we have proceeded parallel to quantum mechanical issues, we have preferred to deliberately use the name “momentum operator” because of the quantum dynamical impressions. However it seems more appropriate to call it “Symmetrized Spatial Differential Operator”. We do not continue focusing on this issue since our purpose here is rather to furnish mathematical structure.

As we obtained (44) and (50) we can construct the expectation dynamical ODEs by using commutator algebra and fluctuation free representation. However this is a technical issue and not necessary to be described in detail here.

The Hamiltonian in (45) produces just a single ODE. However it is possible to replace it with the following extended one to produce a set of ODEs

$$\widehat{H}(t) = \sum_{j=1} \frac{1}{2} \{a_j(\widehat{x}_1, \dots, \widehat{x}_n, t) \widehat{p}_j + \widehat{p}_j a_j(\widehat{x}_1, \dots, \widehat{x}_n, t)\} \tag{51}$$

where \widehat{x} s are independent variable operators while the \widehat{p} s are corresponding symmetrized differentiation operators. This Hamiltonian takes us to the following set of ODEs

$$\dot{\xi}_j(t) \equiv \langle \dot{\widehat{x}}_j \rangle = a_j(\xi_1(t), \dots, \xi_n(t), t), \quad j = 1, 2, \dots, n \tag{52}$$

9 Constructing the probabilistic foundation for a dynamical system

Now we can itemize the steps for constructing a probabilistic foundation for a dynamical system as follows

1. The dynamical system is represented by the ODEs and the accompanying boundary conditions. These can be considered as (52) but with a set of initial values for ξ s;
2. If the given set of ODEs are not autonomus then, by defining a new unknown $\xi_{n+1}(t) \equiv t$, the number of the equations and the initial conditions is increased by 1. Now all right hand side functions become explicitly dependent on ξ_{n+1} instead of t . This creates the autonomus structure and facilitates all the subsequent steps. However it is not a necessity. Depending on the analytical demands the nonautonomus form may even be preferred;
3. ξ s are considered as the expectation values of the algebraic operators separately defined for each independent variable like \widehat{x}_j for x_j . These may be called “Position operators”;
4. We symbolize the j th symmetrized differentiation operator, which takes derivative with respect to x_j and then multiples the result by $-i$, \widehat{p}_j by following the quantum dynamical conceptuality. We removed the reduced Planck constant factor since it does not appear explicitly in the Hamiltonian;
5. We consider the Hamiltonian given in (51) and use its wave function for the expectations. However we never need the wave function explicitly. This does not mean the wave functions remain arbitrary. It does satisfy

$$i \partial \psi(x_1, \dots, x_n, t) \partial t = \widehat{H} \psi(x_1, \dots, x_n, t) \tag{53}$$

where \hbar is removed since they cancel out with the \hbar s of the \widehat{p} s when this equation is written as an explicit PDE;

6. Equation (53) defines an evolution and the initial form of the wave function may be temporally changing depending on the a functions. This makes the initial form

quite important. First of all, it must be designed in such a way that the initial values of each position must be equivalent to the imposed values as accompaniments to the ODEs. The spread, the height and some other parameters of the initial wave form must be compatible with the theoretical background of the dynamical system model and must be consistent with the practical issues;

7. The Hamiltonian is expanded to powers of position operators. This enables us to evaluate the previously defined H functions which become real values because of the provided autonomous structure which makes the Hamiltonian time invariant;
8. The matrix C of the previous section or its upper leftmost truncations are evaluated;
9. By using the result of the previous item, the obtained linear set of ODEs over the expectation of the basis operators of previous section is solved. Since the coefficient matrix is constant the ODE set can be even analytically solved. This infinite linear vector differential equation comes from the probabilistic considerations. Hence we can call it “Probabilistic Evolution Equation” of the dynamical system under consideration. On the other hand, the same equation can also be considered as an unfolded form of the ODEs characterizing the dynamical system since all expectation powers are replaced by single expectations of appropriate powers;
10. The solution obtained in the previous item determines the expectations of the basis operators at least approximately (for the truncated finite set case). This enables us to determine the fluctuations. Since the fluctuations are basically affected by uncertainties in the initial values they can be used to understand how the errors propagate in time during the evolution of the dynamical system under consideration.

10 Concluding remarks

This paper takes comprehensive look at earlier research [13] to show that it is possible to construct a probabilistic wave evolution such that the expectations of a complete operator basis set are evaluated by using the wave function of this evolution. The Hamiltonian of the evolution is determined such that the expectation dynamical equations for the position operators give the dynamical system equations within the fluctuation free representation limit. Hamiltonian is found to be rather simple and related to the vector fields in fact. The infinite linear set of ODEs in the expectation dynamical equations can be analytically solved as long as the dynamical system under consideration is autonomous. This is an important development since it takes us to the realm of linear set of ODEs where a lot of tools in the linear vector space can be used. Especially an efficient stability analysis can be developed through the spectral analysis of the coefficient matrix of this ODE set.

The infinite number in the expectation dynamics may be considered awkward here. We have used the powers of the \hat{x} s and \hat{p} s. This comes from an impression from the Taylor or Maclaurin series and it is not mandatory to use this basis set. Any other complete set of basis operators could have been proposed. The resulting expectation dynamics would be again in infinite number. However depending on the commutation relations with the Hamiltonian the coefficient matrix may be in lumped or block

structured form to facilitate the further analysis. In other words, the selection of the basis set operators is an important issue. It is worthy studying.

The word “Hamiltonian” have been used because of the impressions from quantum mechanics. There is no direct analogy to mechanical concepts unless some limitations related to \widehat{p} are considered. The evolution operator is more meaningful.

The basis set can be squeezed by discarding all elements containing \widehat{p} since there is no natural role of this operator in formulae except in the structure of the evolution operator. It vanishes from the expectation equations unless we want to add the terms containing this operator. The situation is much simpler than we thought.

As it was shown in some papers [14, 15] of the first author it is possible to convert an ODE set, even when it is nonlinear, to set of quadratic ODEs as long as certain closedness conditions like the one under the gradient are fulfilled by the a functions. This makes it attractive to deal with quadratic ODE sets in the framework of this paper.

It is possible to convert the infinite linear equations (probabilistic evolution equation) to an infinite matrix ODE whose solution is initialized by the unit operator. In other words, the propagator concept may separate the initial conditions.

As we have mentioned, the probabilistic evolution equation is in fact composed of folvecs (folded vectors) and folmats (folded matrices). Although we have preferred to unfold all these entities to be able to use ordinary linear algebraic concepts, it is also possible to directly deal with these folarrs (folded arrays). Especially some decomposition methods [16–22] like the Singular Value Decomposition [23–39] can be used to facilitate the employment of these entities.

Here we get first degree \widehat{p} dependence in \widehat{H} to get dynamical equations in $\dot{\mathbf{x}}(t) = a(\mathbf{x}(t))$ form. If we would take this dependence second degree then we would get dynamical equations in $\ddot{\mathbf{x}}(t) = a(\mathbf{x}(t))$ form as we get in quantum dynamics. The higher \widehat{p} dependence in \widehat{H} , the higher differentiation order in the resulting ODE set form.

The companion of this paper will be on the phenomenological reasoning of the probabilistic approach proposed here as well as certain application possibilities on dynamical causal modelling in neuroscience.

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