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ORIGINAL PAPER

Probabilistic evolution approach to the expectation value dynamics of quantum mechanical operators, part II: the use of mathematical fluctuation theory

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Abstract The first part of these two companion papers has been devoted to the extension of Hausdorff moment problem to the sequences over integrals of Kronecker powers of an appropriate vector under a generating function in the kernel. The relations between this generating function and weight function properties have been investigated over there in a quite detailed manner. This second companion paper focuses on the utilization of the "mathematical fluctuation theory" amenities in the construction of approximations to the solutions of the expectation value dynamics of the quantum dynamical systems. The fluctuation freee approximation matching with the classical mechanical behaviour is followed by the first and then the second order fluctuation approximations. Beside the well known "Energy Conservation Law"s counterparts in these approximations of quantum expectation value dynamics are also presented.

Keywords Probabilistic evolution approach · Quantum mechanics · Ehrenfest Theorem · Expectation value dynamics · Kronecker power series · Mathematical fluctuation theory · Quantized Hamilton dynamics · Quantal cumulant dynamics

Mathematics Subject Classification 15A18 · 34A05 · 34A12

1 Introduction

The first one of these two companion papers has a quite detailed introduction why this study has been realized. In fact, the basic foci of these papers are (i) Expectation value

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dynamics for the evolution of quantum systems; (ii) Recently developed probabilistic evolution approach (PEA), to be utilized in the solution of the ODEs for the expectation values certain operators and their powers; (iii) Moment problem like issues for getting integral representations for obtaining uniform convergence in Kronecker power series appearing in (ii). The basic important issues related to PEA have been in the first companion within a sufficiently comprehensive detailing although the interested reader can find an abundance of papers [8–16] in scientific literature. The moment related issues have been the core part of the companion paper. Important results are reported there even in the theorem format. We are not going to refocus on these issues here. However we highly recommend that the first paper should be kept close when this paper is under consideration, to get quick references, since we do intend not to repeat the related issues existing there but to refer certain formulae and paragraphs over there.

The main focus of this paper is to use a new concept of last decade, called the mathematical fluctuation theory developed and have been used extensively in recent years by M. Demiralp and his group members. This is done in a novel approach by developing an expansion which is based on the ascending powers of certain so-called fluctuation operators. This enables us to work in subspaces spanned by certain operators of the set spanning the entire space used in the commutator algebra through Poission brackets with the system's Hamiltonian for the expectation value dynamics of the quantum system under consideration.

After this brief introduction, the remaining part of the paper is organized as follows. Section 2 gives a few core points of the mathematical fluctuation theory. The novel approach which may be somehow called the "Theory of Fluctuation Expansions" is discussed in Sect. 3. Section 4 covers one of the most important property of the Theory of Fluctuation Expansions, which proposes specific energy and fluctuation conservation laws. The confirmation of the classical limit with the proposed method given in Sect. 5, while Sect. 6 deals with the phase or state space considerations. Section 7 is devoted to the application of the proposed method to an example system, symmetric quartic anharmonic oscillator, and the giving numerical results. The paper will be finalized by some further concluding comments and remarks for future directions as usual.

2 The mathematical fluctuation theory

The mathematical fluctuation concept finds its roots in the noncommutativity of the powering and expectation value taking operations. In a simple way we can emphasize on the fact that "the expectation value of a function's or variable's square is not equal to the square of its expectation value unless very specific conditions are satisfied. In mathematical language

$$\int_a^b dx\, W(x) f(x)^2 \neq \left(\int_a^b dx\, W(x) f(x) \right)^2 , \qquad \int_a^b dx\, W(x) = 1 \tag{1}$$

where W stands for a given weight function which can vanish only a finite number of points in the interval, and, we implicitly assume that we are dealing with only

real-valued entities. Otherwise, the expectation value should be redefined appropriately. The relation between the integrals in (1) may not be immediately noticed at the very first glance. However, each integral can be considered as the expectation value of either $f(x)$ or its square with respect to the unit constant basis function under the weight W if and only if the integral of the weight function, which may be considered as the expectation value of the unit operator, is 1. This is the reason why we impose the unit integral condition over the weight function.

Equation (1) is given for continuous functions given on intervals. However, it is possible to deal with the functions with discrete domains. In those cases, the weight function should be replaced by an indexed entity which can take only positive values for its all index values. On the other hand, there are certain circumstances where the weight function remains positive for all independent variable values and depends on certain parameters such that the weight function approaches to Dirac delta function for some limit values of one or more number of these parameters. This Dirac delta function is not a weight function and even not a function but distribution. It has a very important feature that its integral after multiplying it by a continuous function produces the function's value evaluated at the point in the interval, defined by the support of the delta function, as long as the delta's support remains inside the integration interval. The Dirac delta function is the only function having no fluctuation defined like in (1).

Equation (1) is not the only possibility to mention fluctuation. The following denumerable infinite number of equalities can be used to get practically utilizable fluctuations.

$$\phi_j^{(f)} \equiv \int_a^b dx\, W(x) f(x)^{j+1} - \left(\int_a^b dx\, W(x) f(x) \right)^j \equiv \left\langle \widehat{f}^j \right\rangle - \left\langle \widehat{f} \right\rangle^j ,$$
$$j = 1, 2, \ldots ; \qquad \int_a^b dx\, W(x) = 1 \tag{2}$$

where the superscript (f) is used to emphasize on the fact that the defined fluctuation is with respect to the function f, and we have taken the fact that there is no fluctuation in the zeroth and first powers. The left and right angle symbols are used to denote the expectation value of the entity between them. The overhat symbol has been used to mean that the base is an operator. In this case $\widehat{f}$ stands for the function multiplication operator which multiplies its operand by the function value $f(x)$. We could also define the following fluctations for the independent variables

$$\phi_j^{(x)} \equiv \int_a^b dx\, W(x) x^{j+1} - \left(\int_a^b dx\, W(x) x \right)^{j+1} \equiv \left\langle \widehat{x}^j \right\rangle - \langle \widehat{x} \rangle^j ,$$
$$j = 1, 2, \ldots ; \qquad \int_a^b dx\, W(x) = 1. \tag{3}$$

where $\widehat{x}$ multiplies its operand by x everywhere in the interval. The following equality holds for a function $f(x)$ as long as it remains analytic at every point of the considered interval

$$\left\langle \widehat{f} \right\rangle = \langle f\left(\widehat{x}\right)\rangle = \int_a^b dx\, W(x) f(x) = \sum_{j=0}^{\infty} f_j \int_a^b dx\, W(x) x^j = \sum_{j=0}^{\infty} f_j \left\langle x^j \right\rangle =$$

$$= \sum_{j=1}^{\infty} f_{j+1} \phi_j^{(x)} + f\left(\langle \widehat{x} \rangle\right), \qquad \int_a^b dx\, W(x) = 1. \quad (4)$$

If the weight function is sufficiently sharply located around an interval point then the fluctuations can be considered rather small, and then, they can be omitted. What we call this omittance case is "Fluctuationlessness Approximation" and write

$$\langle f\left(\widehat{x}\right)\rangle \approx f\left(\langle \widehat{x} \rangle\right) \quad (5)$$

This approximation equality may not be so strong because of it is defined to a rather simple function, the unit constant function. However the above analysis can be repeated over a finite number of basis function whose the very first one is the unit constant function then the expectation values are replaced by the matrix representations of the operators. Even though we do not intend to give all intermediate details we can write the approximation equality as follows

$$\mathbf{M}^{(\mathcal{U}_n)}\left(\widehat{f}\right) \approx f\left(\mathbf{X}^{(\mathcal{U}_n)}\right) \quad (6)$$

where

$$\mathcal{U}_n \equiv \left\{u_j(x)\right\}_{j=1}^{j=n}, \qquad u_1(x) \equiv 1x \in [a, b,], \quad \mathbf{u}_n(x) \equiv [u_1(x) \quad \ldots \quad u_n(x)] \quad (7)$$

and u_j functions are mutually orthogonal with unit norms. Beyond these the following definitions are also valid

$$\mathbf{M}^{(\mathcal{U}_n)}\left(\widehat{f}\right) = \int_a^b dx\, W(x) \mathbf{u}_n(x) f(x) \mathbf{u}_n(x)^T,$$

$$\mathbf{X}^{(\mathcal{U}_n)} = \int_a^b dx\, W(x) \mathbf{u}_n(x) x \mathbf{u}_n(x)^T \quad (8)$$

These are matrix equations and define $n \times n$ elements for each representation. Equation (6) is also a matrix approximation equality over $n \times n$ elements. It becomes exact when n goes to infinity as long as the set $\mathcal{U}_\infty$ spans the Hilbert space where the expectation values reside. Hence, the greater the n value the greater the approximation quality. Equation (6) is the core subject of the so-called Fluctuationlessness Theorem which

was conjectured and proven by M. Demiralp. It has been successfully utilized in many practical applications by Demiralp's group members [3,5–7]. It was first given for univariate functions. Later, its multivariate version [4] has also been conjectured and proven by M. Demiralp again.

Further investigations on mathematical fluctuations have also been realized and some interesting findings were reported. We find this information as a gentle introduction to "mathematical fluctuation theory" sufficient for our purposes here. The next section contains for various detailing of fluctuation expansions in the expectation value dynamics for quantum systems.

3 The theory of fluctuation expansion for quantum expectation value dynamics

Even though the basic philosophy we are going to use here were visited many times, but generally for different purposes and within different point of views in the scientific literature [17–19]; the fluctuationlessness approximation for the expectation value dynamics of a quantum system produces a set of ordinary differential equations (ODE) where the number of the unknown temporal functions is equal to the twice of the degree of the freedom in the system under consideration. To be able to describe details we first recall Ehrenfest Theorem [2] that connects classical mechanics and quantum mechanics to certain extend.

We focus on a one dimensional system where the position variable x takes values from the real number set. We will keep the presentation somehow general at the beginning to be ready for dealing with any system which fits to the limitations of the presentation. The system under consideration, is completely described by two operators, momentum operator $\widehat{p}$ and position operator $\widehat{q}$. The position operator's action on a function $f(x)$ depending on the position variable x is defined as follows

$$\widehat{q} f(x) \equiv x f(x), \qquad x \in (-\infty, \infty) \tag{9}$$

where the position variable plays the role of the eigenvalue of the position operator. For systematic consideration it is better not to confuse these two entities: position operator $(\widehat{q})$ and the position variable (x). x plays the role of a dummy variable in the mathematical sense while the position operator $\widehat{q}$ truely describes the positioning of the particle in the system and the observed numerical values are related to this operator through its expectation value.

The momentum operator $\widehat{p}$, on the other hand, is defined through the spatial differentiation (the differentiation with res pect to position variable x). Its explicit definition is given by

$$\widehat{p} f(x) \equiv -i\hbar \frac{\partial f(x)}{\partial x}, \qquad x \in (-\infty, \infty)\,. \tag{10}$$

Here and in (9) $f(x)$ is assumed to be lying in the Hilbert space where the wave function of the system resides. Hence, it should satisfy the conditions for continuity and square integrability over all position values. The symbol $\hbar$ stands for the "Reduced

Planck Constant" which is the ratio of the ordinary Planck constant to 2π. That constant somehow enters the uncertainty and therefore probability issues. As it tends to decrease the system under consideration behaves more classical mechanically and the probability density tends to be sharp such that it approaches Dirac delta function type structure in the vanishing Planck constant limit which is mathematically inaccessible because of the nonzero true value of the Planck constant. However, the dimensional entities may climb to the large values in comparison with the realm of the atoms and molecules, by taking the system to the macro level where classical mechanical rules govern the system.

The Hamilton operator $\widehat{H}$ of the one dimensional quantum system is defined as follows in terms of the momentum and position operators

$$\widehat{H} \equiv \frac{1}{2\mu}\widehat{p}^2 + V\left(\widehat{q}\right) \tag{11}$$

where μ denotes the mass of the system's particle which can move only in a line where the location is represented by x. The potential function V is assumed to be analytic on the real axis of x except the infinity. The Hamilton operator has no explicit time dependence, and therefore, it is autonomous. The Hamilton operator autonomy defines a system which has no interaction with its environment. In other words, we confine ourselves to the isolated systems.

The momentum and position operators are self-adjoint (Hermitian) as long as the wave function of the system sufficiently rapidly decays to annihilate the residual terms of the integration-by-parts operation. This Hermiticity implies the self-adjointness of the Hamilton operator. The Hermiticity of the operators guarantee the real valued ness of their expectation values. All operators considered for the quantum systems are linear by definition and map from the Hilbert space where the wave function lies to the same space.

The expectation value of an operator, which may explicitly vary in time and denoted by $\widehat{o}(t)$ is defined as follows

$$\begin{aligned}\langle\widehat{o}(t)\rangle &\equiv (\psi(t), \widehat{o}(t)\psi(t)) \\ &\equiv \int_{-\infty}^{\infty} dx\, \psi(x,t)^* \widehat{o}(t)\psi(x,t)\end{aligned} \tag{12}$$

where the first identity states that the expectation value of an operator is equivalent to the innerproduct of the wave function's image under the considered operator with the wave function and the spatial dependence of the wave function has not been shown explicit ly since x is the dummy variable of the innerproduct integration. The second identity expresses the innerproduct more explicitly.

Despite the expectation value is based on the wave function we can avoid its explicit utilization by forgetting the explicit structure of the definition but constructing an ordinary differential equation (ODE). The temporal differentiation of the both sides of the expectation value definition permits us to write the following equation by skipping the intermediate steps

$$\frac{d\,\langle\widehat{o}(t)\rangle}{dt} = \langle\{\widehat{H},\widehat{o}(t)\}\rangle + \left\langle\frac{d\widehat{o}(t)}{dt}\right\rangle \tag{13}$$

where the expression whose expectation value is taken at the right hand side's first additive term is well-known and called "Poisson Bracket". Its explicit definition is given below

$$\{\widehat{H},\widehat{o}(t)\} \equiv \frac{i}{\hbar}\left[\,\widehat{H}\widehat{o}(t) - \widehat{o}(t)\widehat{H}\,\right] \tag{14}$$

which is apparently self-adjoint because of the proportionality constant of the commutator between $\widehat{H}$ and $\widehat{o}(t)$, despite the commutator is anti Hermitian. The derivation of (13) is not hard although we have skipped the details, and, is based on the Schrödinger equation and its complex conjugate we have not given explicitly here.

Now, by skipping the intermediate steps again, we can obtain the following equations for the expectation values of the momentum and position operators.

$$\begin{aligned}\frac{d\,\langle\widehat{p}\,\rangle(t)}{dt} &= -\langle V(\widehat{q})\rangle(t)\\ \frac{d\,\langle\widehat{q}\,\rangle(t)}{dt} &= \frac{1}{\mu}\langle\widehat{p}\,\rangle(t).\end{aligned} \tag{15}$$

The right hand side of the first one of these equations is not directly expressible in terms of position and momentum operators only. Instead, the natural number powers of the position operator enter the expectation value if we use the Taylor series expansion of the potential function. Since the expectation value of an integer power of the position operator can not be expressed in terms of the position and momentum operator expectation values only, the two equations in (15) do not form a complete set of ODEs. This incompleteness urges us to construct more equations by involving the expectation values of the position operator integer powers until the resulting set of ODEs becomes complete. However this procedure ends in a denumerably infinite set of ODEs as we have shown quite recently when we develop the "Probabilistic Evolution Equations"[12–14]. On the other hand it is very well known that any given operator related to the system under consideration approaches to the unit operator multiplied by the expectation value of that operator at the classical limit where the probability density approaches Dirac delta function like sharp single peak (or "distribution " in more mathematical terminology). This leads us to use not the operator's itself but its deviation from the unit operator multiplied by its expectation value. To this end, we can write the following equality for an operator $\widehat{o}$ which is autonomous

$$\widehat{o} = \langle\widehat{o}\,\rangle(t)\widehat{I} + \widehat{\varphi}_o(t), \qquad \widehat{\varphi}_o(t) \equiv \widehat{o} - \langle\widehat{o}\,\rangle(t)\widehat{I} \tag{16}$$

where the subscript o implies the relation to the operator $\widehat{o}$. We call the operator $\widehat{\varphi}_o(t)$ "Fluctuation Operator for $\widehat{o}$". This decomposition presented here is the natural decomposition and called "moving frame approach" in scientific literature [17,18], due to the fact that the potential function will be presented with a series expansion around

a point. This series expansion is time dependent because of the time dependence of the fluctuation operator. Thus, it is natural to select expansion as average position at the current time. However, this operator decomposition is not unique. This decomposition can also be considered as the projection of the operator under consideration to two different subspaces of the all space. This decomposition can be defined by an optimization algorithm that reduces the magnitude of the fluctuation in the evolving time.

We can now expand the Potential Function's first derivative over the position operator around the unit operator multiplied by the expectation value of the position operator as follows

$$V'\left(\widehat{q}\right) = \sum_{j=0}^{\infty} (j+1) V_{j+1}\left(\langle \widehat{q} \rangle (t)\right) \widehat{\varphi}_q(t)^j \tag{17}$$

where the zero power of the fluctuation operator is assumed to be unit operator by following the operator algebraic convention on operators.

By using the linearity in the expectation value taking operation we can write

$$\left\langle V'\left(\widehat{q}\right)\right\rangle (t) = \sum_{j=0}^{\infty} (j+1) V_{j+1}\left(\langle \widehat{q} \rangle (t)\right) \left\langle \widehat{\varphi}_q(t)^j \right\rangle \tag{18}$$

where we have not shown the expectation value dependence on time when it is unnecessary. The convergence of the above series is one of the key points of the presented method. For the potentials that converge slowly , such as exponential potential like Morse potentials with certain parameters, more terms are needed for a prescribed quality. This certainly increases of the computational effort. On the other hand, for the potentials having singular points in the computational domain this series may diverge that lead to divergence and/or non-stable solutions of the presented method. To be able to overcome this issues, different types of series expansions which takes polynomials as the basis set such as Chebyshev polynomials can be considered to accelerate the convergence rate. For the divergent potentials, Laurent series can be considered with the redefinition of the studied operator space. Further details are given in the following sections.

To proceed, it is possible to write the following equations, recalling back the above series expansion and utilizing the Ehrenfest Theorem in Heisenberg picture.

$$\frac{d\left\langle \widehat{\mathbf{s}} \right\rangle (t)}{dt} = \sum_{j=0}^{\infty} \mathbf{H}_j \left\langle \widehat{\mathbf{s}}^{\otimes k} \right\rangle, \quad j = 0, 1, 2, \ldots \tag{19}$$

Here, $\mathbf{H}_j$ denotes an $n \times n^j$ dimensional rectangular matrix and its dimension changes depending on the system under consideration and the defined system vector $\widehat{\mathbf{s}}$. n is the number of operators included in $\widehat{\mathbf{s}}$. The structure of the system vector and thus the number of elements can be changed to be able to get the desired structure in the evolution matrix as described in the previous chapter. Another important point is that

these matrices are time invariant. Thus, the above system of equations are linear in expectation value of $\widehat{\mathbf{s}}$ and its Kronecker powers. Taking this linear set of ODEs in one hand, we will now utilize the "Theory of Fluctuation Expansion". For this purpose, we first define "fluctuation vector" using previously defined operator decomposition as follows.

$$\widehat{\phi}(t) = \widehat{\mathbf{s}} - \langle \widehat{\mathbf{s}} \rangle (t)\widehat{\mathbf{I}} \tag{20}$$

$$\widehat{\mathbf{s}} = \langle \widehat{\mathbf{s}} \rangle (t)\widehat{\mathbf{I}} + \widehat{\phi}(t) \tag{21}$$

In these equations $\widehat{\mathbf{s}}$ denotes the system vector composed of the operators describing the system under consideration in PEA perspective; while $\widehat{\phi}(t)$ stands for the portions of these operators, which causes fluctuations. As can be explicitly noticed from these equations, the expectation value of the operator $\widehat{\phi}(t)$ during the entire time interval where the dynamics is investigated is zero.

$$\left\langle \widehat{\phi}(t) \right\rangle = 0 \tag{22}$$

The efficiency of the decomposition in (21) will be shown in the coming steps as we proceed. However, this does not mean that the identity in (21) is the only possible identity. The other decompositions whose first components have the value of the expectation value, $\langle \widehat{\mathbf{s}} \rangle (t)$ while the second component is an operator whose expectati on value vanishes.

More complicated ideas can be brought to the scene for the above mentioned decomposition. However, the increasing complications the growing efforts to proceed efficiently. For instance, different probability distributions may be involved in the procedure and produce different efficiencies. The present approach has been chosen to expect better efficiency by keeping the zero reduced Planck constant limit as the classical mechanics.

Before using these notions in the expectation value dynamical equations, we need to investigate how the expectation values of the fluctuation operators are reflected to the expectation values of the system vector's Kronecker powers. The first step to this end is to focus on the Kronecker square expectation value of the system vector.

$$\widehat{\mathbf{s}}^{\otimes 2} = \langle \widehat{\mathbf{s}} \rangle (t)^{\otimes 2}\widehat{\mathbf{I}} + \langle \widehat{\mathbf{s}} \rangle (t)\widehat{\mathbf{I}} \otimes \widehat{\phi}(t) + \widehat{\phi}(t) \otimes \langle \widehat{\mathbf{s}} \rangle (t)\widehat{\mathbf{I}} + \widehat{\phi}(t)^{\otimes 2} \tag{23}$$

$$\left\langle \widehat{\mathbf{s}}^{\otimes 2} \right\rangle (t) = \langle \widehat{\mathbf{s}} \rangle (t)^{\otimes 2} + \left\langle \widehat{\phi}(t)^{\otimes 2} \right\rangle \tag{24}$$

We call the case where all terms coming from fluctuations are neglected, "Fluctuationlessness Approximation". Even though this is just for the Kronecker square of the system vector expectation value. However, it can be extended to the all positive integer Kronecker powers. By skipping the intermediate details we can write the more general extended equation as follows

$$\left\langle \widehat{\mathbf{s}}^{\otimes j} \right\rangle (t) \approx \langle \widehat{\mathbf{s}} \rangle (t)^{\otimes j}, \qquad j = 2, 3, \ldots \tag{25}$$

This approximation leads to the classical limit equations of motions what we called "fluctuationless limit".

$$\frac{d\,\langle\widehat{\mathbf{s}}\rangle\,(t)}{dt} = \sum_{j=0}^{\infty} \mathbf{H}_j\,\langle\widehat{\mathbf{s}}\rangle\,(t)^{\otimes j} = \mathbf{R}_0(\langle\widehat{\mathbf{s}}\rangle\,(t)), \tag{26}$$

After all these steps, to be able to mathematically describe the full approximation of the proposed algorithm, first we will recall an important property of the Kronecker product

$$\widehat{\mathbf{y}} \otimes \widehat{\mathbf{x}} = \Sigma(\widehat{\mathbf{x}} \otimes \widehat{\mathbf{y}}) \tag{27}$$

where Σ denotes the unitary permutation matrices whose columns and rows are appropriately chosen unit vectors. Using this property, the Binomial Expansion of the nth Kronecker power of the sum of two vectors can be explicitly written in the following form.

$$(\widehat{\mathbf{x}} + \widehat{\mathbf{y}})^{\otimes j} = \sum_{k=0}^{j} \Sigma_k(\widehat{\mathbf{x}}^{\otimes k} \otimes \widehat{\mathbf{y}}^{\otimes j-k}) \tag{28}$$

Utilizing the above equations, Poisson brackets for the fluctuation vector and the conservations rules which will be discussed in the following chapter we get the following linear systems of ordinary differential equations.

$$\begin{aligned} \frac{d\,\langle\widehat{\mathbf{s}}\rangle\,(t)}{dt} &= \sum_{j=0}^{\infty} \mathbf{R}_j(\langle\widehat{\mathbf{s}}\rangle\,(t))\varphi_j(t) \\ \frac{d\varphi_j(t)}{dt} &= \sum_{k=0}^{\infty} \rho_{j,k}(\langle\widehat{\mathbf{s}}\rangle\,(t))\varphi_k(t) \\ & \qquad j = 1, 2, 3, \ldots \end{aligned} \tag{29}$$

In the above equations the term $\varphi_j(t)$ must be considered as follows

$$\varphi_j(t) = \left\langle \widehat{\phi}(t)^{\otimes j+1} \right\rangle \tag{30}$$

The Eq. (29) is the hearth of the proposed method. ODEs written for the fluctuation terms are denumerably infinite. One way to deal with these equation is the PEA and its given in the accompanying paper [1]. Another way to deal with these equations are truncation approximations. For instance, the zeroth order truncation so called fluctuationless limit corresponds to the classical limit. The accuracy will be better when the more terms are involved in the truncation approximants. The convergence rate will depend on the system under consideration and strongly related to the convergence rate of the potential function of the system. Due to the probabilistic nature of the quantum systems, we are unable to discuss the uniform convergence. The convergence is in a

strong correlation with the width of the initial wave packet and its velocity spreadth. If the the width and the velocity is small, then the convergence and the accuracy of the presented method will be good in a large time interval. But if the width and spread velocity is not small enough, the method will give good approximations only in the very small time intervals. But truncating in large number of terms will overcome this issue within an asymptotic convergence.

4 Conservation rules via the theory of fluctuation expansion

This section covers the conservation laws in fluctuation expansions for the symmetric quartic anharmonic quantum oscillator. We are going to keep the investigations at general level as much as possible. The basic idea for this investigation is the fact that the expectation value of the Hamilton operator remains constant during the entire evolution of the system as long as the Hamiltonian is autonomous. The time variation of the Hamilton operator's expectation value can be given through the following equations.

$$\begin{aligned} \frac{d\left\langle \widehat{H}\right\rangle}{dt} &= \left\langle \left\{ \widehat{H}, \widehat{H} \right\} \right\rangle = 0 \\ \left\langle \widehat{H}\right\rangle &= \frac{1}{2\mu}\left\langle \widehat{p}^2 \right\rangle + \left\langle V\left(\widehat{q}\right)\right\rangle = H_0 \end{aligned} \tag{31}$$

H_0 denotes a scalar in the last equation of (31) For further proceeding we need to focus on the momentum and position operators and related fluctuation operators. In fact, our main purpose is to determine the expectation values of these entities and then to find the evolution of the quantum dynamical systems via probabilistic evolution approach.

$$\begin{aligned} \widehat{\Phi}_p &\equiv \widehat{p} - \left\langle \widehat{p}\right\rangle \widehat{I} \\ \widehat{\Phi}_q &\equiv \widehat{q} - \left\langle \widehat{q}\right\rangle \widehat{I} \end{aligned} \tag{32}$$

We need to reemphasize on the fact that the expectation values of the fluctuation operators vanish. The other important issue is the possibility of decomposing a given operator to two components, in any way, as long as the expectation value of whose first component should match the expectation value of the operator under consideration while the second component's expectation value vanishes. The first preferable way is the development a method such that the first approximation aims at the fluctuationless limit while the other approximations gradually involves the ascending degrees of the fluctuations as the corrections. In this perspective some inspiration can be taken Wigner function related issues. The series expansion of the potential function can be given as follows

$$\left\langle V\left(\widehat{q}\right)\right\rangle = \sum_{j=0}^{\infty} v_j \left\langle \widehat{q}^j \right\rangle \tag{33}$$

The explicit structure of $\widehat{q}^j$ operators can be written as follows in terms of fluctuation operators

$$\widehat{q}^{\,j} = \left(\langle \widehat{q} \rangle \, \widehat{I} + \widehat{\Phi}_q\right)^j = \sum_{k=0}^{j} \binom{j}{k} \langle \widehat{q} \rangle^k \, \Phi_q^{j-k} \tag{34}$$

where we can define

$$\varphi_{j-k-1,q^{j-k}}(t) = \left\langle \Phi_q^{j-k} \right\rangle \tag{35}$$

and use in (33) to get the following result

$$\langle V(\widehat{q}) \rangle = \sum_{j=0}^{\infty} \left(\sum_{k=0}^{\infty} \binom{j+k}{k} v_k \, \langle \widehat{q} \rangle^k \right) \varphi_{j-1,q^j}(t). \tag{36}$$

The expectation value of the momentum operator square in terms of the fluctuation operators as follows

$$\left\langle \widehat{p}^2 \right\rangle = \langle \widehat{p} \rangle^2 + \varphi_{1,p^2}(t) \tag{37}$$

If all these findings are used in the second equality of (31) then the following conservation law can be written

$$\frac{1}{2\mu} \langle \widehat{p} \rangle^2 + V(\langle \widehat{q} \rangle) + \varphi_{1,2} + \sum_{j=0}^{\infty} \frac{V^{(j+1)}(\langle \widehat{q} \rangle)}{(j+1)!} \varphi_{j,0} = H_0 \tag{38}$$

where

$$\varphi_{j,k} \equiv \left\langle \frac{1}{2} \widehat{\Phi}_p^k \widehat{\Phi}_q^{j+1-k} + \widehat{\Phi}_q^{j+1-k} \widehat{\Phi}_p^k \right\rangle, \quad j = 1, 2, \ldots; \quad k = 0, 1, \ldots, j+1 \tag{39}$$

should be kept in mind.

By using these results it is possible to construct conservation laws, which are valid for all time instances during the system's evolution, over the higher degree fluctuation terms. We find this analysis sufficient here.

5 Fluctuation free approximation

Equation (18) takes the following form when all expectation values over all fluctuation (the terms corresponding to the cases where j is positive) are ignored

$$\left\langle V'(\widehat{q}) \right\rangle(t) = V'(\langle \widehat{q} \rangle(t)) \tag{40}$$

which affects (15) as follows by removing the incompleteness between the ODEs via fluctuationlessness approximation

$$\frac{d\left\langle \widehat{p}\right\rangle (t)}{dt}=-V\left(\left\langle \widehat{q}\right\rangle (t)\right)$$
$$\frac{d\left\langle \widehat{q}\right\rangle (t)}{dt}=\frac{1}{\mu}\left\langle \widehat{p}\right\rangle (t). \tag{41}$$

We can now define

$$\xi(t)\equiv\left\langle \widehat{p}\right\rangle (t),\qquad \eta(t)\equiv\left\langle \widehat{q}\right\rangle (t) \tag{42}$$

and rewrite (41) as follows

$$\begin{array}{l}\dot{\xi}=-V'(\eta),\ \xi(0)=\xi_0\\ \dot{\eta}=\frac{1}{\mu}\xi,\qquad \eta(0)=\eta_0\end{array}. \tag{43}$$

which can be converted into a single but second order ODE with accompanying initial conditions

$$\ddot{\eta}=-\frac{1}{\mu}V'(\eta),\qquad \eta(0)=\eta_0,\ \ \dot{\eta}(0)=\frac{1}{\mu}\xi_0 \tag{44}$$

If the first equation of (44) is multiplied by $\dot{\eta}$ and then temporally integrated we obtain

$$\frac{\mu}{2}\dot{\eta}^2+V(\eta)=\frac{1}{2\mu}\xi_0^2+V(\eta_0)\equiv H_0 \tag{45}$$

which states the energy conservation and hence we denoted the integration constant by H_0 to imply the beginning value of the Hamilton operator expectation value at fluctuation free level.

Equation (45) can be further handled by the separation of variables and this results in

$$\mathcal{F}(\eta)\equiv\int_{\eta_0}^{\eta}\frac{d\eta_1}{\sqrt{\frac{2H_0}{\mu}-\frac{2}{\mu}V(\eta_1)}}=t \tag{46}$$

where we assumed that the integration interval does not contain any branch point or some other singularity of the square root in the denominator. This equality states t in terms of η and it is possible to use inverse function of $\mathcal{F}$ as long as it exists to express η in terms of t.

6 Phase space or state space considerations

In classical dynamics the entities describing the system are the position and momentum variables which are temporally varying. The main focus is the determination of these entities. This is an explicit way to find the dynamical behavior of the considered system. However, this task may not be so easy as it appears at the first glance, depending

on the mathematical complications of the governing equations. One can avoid this task to get more global dynamical feature by using rather qualitative or geometrical considerations. To this end, a multidimensional space where each point's coordinates are determined by the system variables, positions and momenta, is defined. This is called "phase space" where the state of the system is represented by a point which moves in this space as the time evolves. The location of these points composes a curve which is called "trajectory". In the framework of system theory, the position and momentum discrimination may not be necessary and all temporal unknowns are considered equivalent to characterize the system and their role dominancy can be understood either after the solution of the dynamical equations or by looking their relative changes. So, these entities which are called "state variables" span again a space which is almost identical to the phase space. This space is called "state space".

It is generally possible to find whether the system under consideration, evolves in a periodical motion (somehow metastability, vibration), or explodes (instability), or decays after initial transitions at the infinite limit of time.

The periodical motions generally correspond to the closed or asymptotically closed trajectories in phase or state space even though certain open curves like parabolas which can in fact be considered as the closed curves in not finite but infinite regions may allow periodical motions. The closed curves correspond to certain conservation rules like energy conservation in classical dynamics. The asymptotically closed trajectories describe the motion of the systems which interact with their environment at the beginning of the evolution and then, after certain finite time interval the system approaches periodical motion. In this work we will focus on a system which will behave always periodical. The following equation can be derived from (45) and is the mathematical statement of the energy conservation for a one dimensional quantum system at the classical limit

$$\frac{1}{2\mu}\xi(t)^2 + V\left(\eta(t)\right) = H_0 \tag{47}$$

where the time dependence through ξ and η is deliberately shown explicitly to emphasize on the fact that this conservation rule remains valid for all time instances during the evolution. H_0 stands for the initial value of the Hamilton function $H(\xi, \eta)$ which produces the Hamilton operator when its arguments are replaced by the momentum and position operators respectively. The value of H_0 depends on the Hamilton function's structure. It may be positive or positive semi-definite for all possible values of its arguments when the Hamilton operator is positive definite. The Hamilton operator's kinetic energy term which is the momentum square divided by the twice of the particle's mass is certainly nonnegative. However, the potential function may produce negative values depending on the potential structure. If it is nonnegative definite then we become enabled to show that the potential function needs to be bounded from above so does the position variable $\eta(t)$. Equation (47) can be used to get these bounds, depending on the functional dependence of the potential function on the position variable. Equation (47) implies that

$$V\left(\eta(t)\right) \leq H_0. \tag{48}$$

This may or may not produce a finite bound on $\eta(t)$ depending on the η dependence of the potential function.

If the potential function is not positive or positive semi-definite then the energy conservation equation may create certain singularities, especially when $\xi(t)$ is attempted to be expressed in terms of $\eta(t)$. Because of the square root operation a branch point may arise to create a turning point where $\xi(t)$ turns out to be imaginary. This is very possibly originated from the modelling of problems generally. If it happens then it is better to revise the model for the system under consideration appropriately. In this work, a positive semi-definite and monotonous potential function will be taken to the focus.

7 Case study: one dimensional symmetric quartic quantum anharmonic oscillator

7.1 Classical limit: the fluctuation free approximation

We focus on a system composed of just a single particle with a mass μ under the potential defined by the following equation

$$V(x) \equiv \frac{k_1}{2}x^2 + \frac{k_2}{4}x^4, \qquad x \in (-\infty, \infty), \quad k_1, k_2 > 0 \tag{49}$$

which implies

$$\frac{k_1}{2}x_{max}^2 + \frac{k_2}{4}x_{max}^4 = H_0 \tag{50}$$

whose only acceptable root amongst the existing four zeroes is explicitly given below

$$x_{max} = \frac{\sqrt{k_1^2 + 4H_0k_2} - k_1}{k_2} \tag{51}$$

This means that

$$\eta(t) \in \left[-\frac{\sqrt{k_1^2+4H_0k_2}-k_1}{k_2} \, , \, \frac{\sqrt{k_1^2+4H_0k_2}-k_1}{k_2} \right], \quad \xi(t) \in \left[-\sqrt{2\mu H_0} \, , \, \sqrt{2\mu H_0} \right] \tag{52}$$

which imply that the position expectation value oscillates between the endpoints of this interval so does the momentum expectation value between its interval endpoints. These facts and the equations in (43) show that the energy conservation is the trajectory on which the state point moves in a periodical motion.

The function $\mathcal{F}(\eta)$ takes the following integral representation form

$$\mathcal{F}(\eta) \equiv \int_{\eta_0}^{\eta} \frac{d\eta_1}{\sqrt{\frac{2H_0}{\mu} - \frac{k_1}{\mu}\eta_1^2 - \frac{k_2}{2\mu}\eta_1^4}} \tag{53}$$

which can be related to the elliptic integrals via appropriate change of integration variable. Hence, this function does not have an explicit exact form but can be expressed in terms of well-known functions. We do not intend to get into more details of this issue here.

7.2 Second order fluctuation expansion

This subsection is devoted to an example of third order fluctuation approximation for the symmetric quartic anharmonic oscillator. For this purpose, first we will construct equations of motions using Ehrenfest theorem.

$$\begin{aligned}
\frac{d\langle\widehat{p}\rangle(t)}{dt} &= -k_1\langle\widehat{q}\rangle(t) - k_2\left\langle\widehat{q^3}\right\rangle(t) \\
\frac{d\langle\widehat{q}\rangle(t)}{dt} &= \frac{1}{\mu}\langle\widehat{p}\rangle(t)
\end{aligned} \tag{54}$$

Since the expectation value of the cube of position operator is a new unknown, the above equations are not close and hence not solvable either numerically or analytically. But this term can be approximated using the Theory of Fluctuation Expansion as follows.

$$\left\langle\widehat{q^3}\right\rangle(t) \approx \langle\widehat{q}\rangle(t)^3 + 3\langle\widehat{q}\rangle(t)\varphi_{1,3} \tag{55}$$

This approximation includes new fluctuation term and three new differential equations can be constructed from the energy conservation law that dictates us that total energy of the same order fluctuation expansion terms is conserved. The final closed set of ODEs is as follows.

$$\begin{aligned}
\frac{d\langle\widehat{p}\rangle(t)}{dt} &= -k_1\langle\widehat{q}\rangle(t) - k_2(\langle\widehat{q}\rangle(t)^3 + 3\langle\widehat{q}\rangle(t)\varphi_{1,3}) \\
\frac{d\langle\widehat{q}\rangle(t)}{dt} &= \frac{1}{\mu}\langle\widehat{p}\rangle(t) \\
\frac{d\varphi_{1,1}(t)}{dt} &= -(k_1 + 3k_2\langle\widehat{q}\rangle(t)^2)\varphi_{1,2} \\
\frac{d\varphi_{1,2}(t)}{dt} &= -2(k_1 + 3k_2\langle\widehat{q}\rangle(t)^2)\varphi_{1,3} + \frac{2}{\mu}\varphi_{1,1} \\
\frac{d\varphi_{1,3}(t)}{dt} &= \frac{1}{\mu}\varphi_{1,2}
\end{aligned} \tag{56}$$

Accompanying initial conditions of the above set of ODEs can be constructed from the initial wave packet. The wave function characterizes the evolution in the quantum system. For simplicity, our quantum system is composed of a single particle and the degree of freedom is just one. Gaussian Wave Packet where the initial distribution's function form is given in position space, as follows

$$\psi(x,0) = \frac{1}{(2\pi\sigma_x^2)^{1/4}} e^{ip_0x/\hbar} e^{-(x-x_0)^2/4\sigma_x^2} \tag{57}$$

and/or in momentum space as follows

$$\phi(p,0) = \frac{1}{(2\pi\sigma_p^2)^{1/4}} e^{-i(p-p_0)q_0/\hbar} e^{-(p-p_0)^2/4\sigma_p^2} \tag{58}$$

where $\hbar$ stands for the reduced Planck's constant which is taken to be 1 in this study for the sake of simplicity. x and p are corresponding to the position and momentum of the system. x_0 and p_0 are given initial values of the position and momentum which are randomly determined for the computational experiments. Moreover, σ_x and σ_p are the variances of the position and the momentum operators expectation values and satisfy the Heisenberg uncertainty relation.

$$\sigma_x\sigma_p \geq \frac{\hbar}{2} \tag{59}$$

Using the informations above, the accompanying initial conditions for the Gaussian initial wave packet can be constructed as follows.

$$\begin{aligned}
&\langle\widehat{q}\rangle(0) = q_0, \quad \langle\widehat{p}\rangle(0) = p_0 \\
&\left\langle\widehat{\varphi}_{1,1}\right\rangle(0) = \left\langle\widehat{p^2}\right\rangle(0) - \langle\widehat{p}\rangle(0)^2 = \frac{m\hbar w}{2} \\
&\left\langle\widehat{\varphi}_{1,2}\right\rangle(0) = \frac{1}{2}\left[\langle\widehat{pq}\rangle(0) + \langle\widehat{qp}\rangle(0) - 2\langle\widehat{p}\rangle(0)\langle\widehat{q}\rangle(0)\right] = 0 \\
&\left\langle\widehat{\varphi}_{1,3}\right\rangle(0) = \left\langle\widehat{q^2}\right\rangle(0) - \langle\widehat{q}\rangle(0)^2 = \frac{\hbar}{2mw}
\end{aligned} \tag{60}$$

7.3 Numerical experiments

The ODEs constructed in previous subsection can be solved numerically with any suitable method. For the solution, we have used Matlab ode45 routine that uses explicit Runge–Kutta method. The mass of the particle and the reduced Planck constant considered to be one. The constants k_1 and k_2 are considered to be one to guarantee the periodic motion. The quantum mechanical simulations are done with the split operator method using Strang split together with the FFT algorithm with 100 time step at most. The Fig. 1 shows the expectation values of the position changing with time. As clearly seen in the figure, the proposed method produces results in a well agreement with the quantum mechanical simulation in small time interval, even though only the

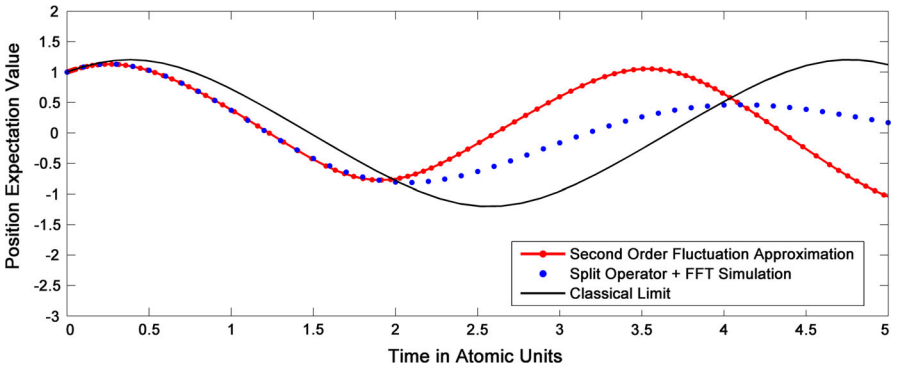

Fig. 1 Comparison of the expectation value of the position operator changing with time ($\sigma_x = 0.5$, $\hbar = 1, m = 1, q_0 = 1, p_0 = 1$)

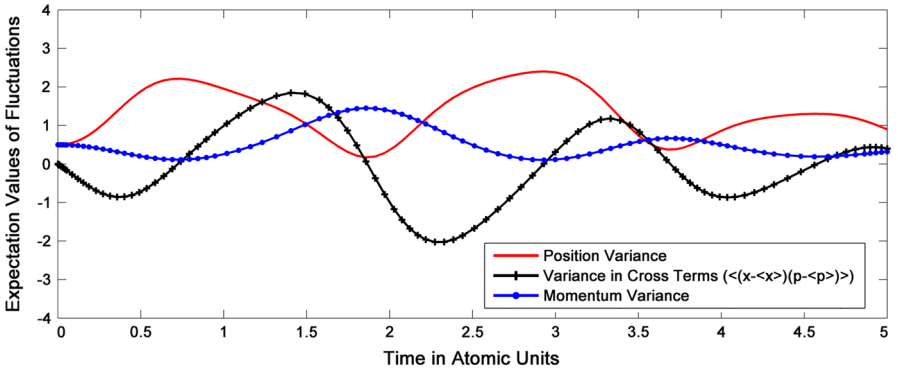

Fig. 2 The expectation values of the fluctuation operators ($\sigma_x = 0.5, \hbar = 1, m = 1$)

second order fluctuation terms are considered. The deviation from the classical limit is also successfully modeled in small time interval. The Fig. 2 shows the expectation values of second order fluctuation operators. The magnitude of the expectation value of the fluctuation operators gets larger as the time evolves due to the fact that the wave function spreads as time passes. The Fig. 3 shows the phase space trajectory of the particle under consideration. In the classical limit, it gets a closed shape as desired but the quantum mechanical corrections by the mathematical theory of fluctuation expansion deviates this closed shape. Moreover, due to energy conservation between the same ordered fluctuation operators the trajectory is still closed. As clearly seen from the figure, the particle moves on the quantum (not classically allowed) region as time evolves. This is because of the fact that the presented method can take quantum effects into consideration.

8 Future perspective: pseudo expectation values

It is important to note that primary step of the presented method is series expansion of the potential function of the system under consideration. However, Taylor series

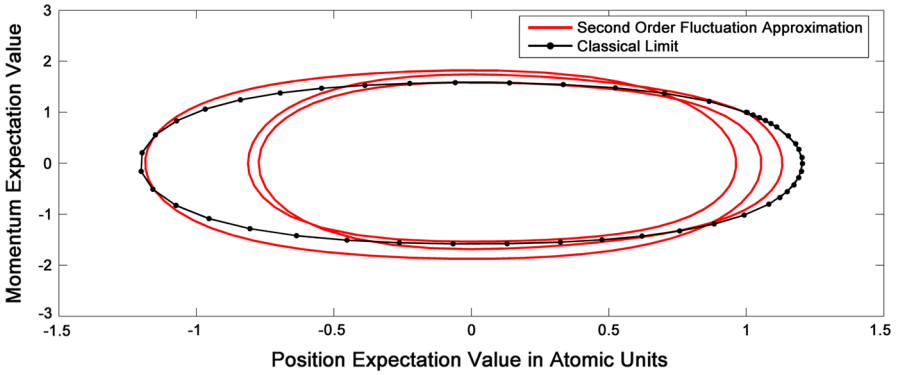

Fig. 3 The phase space of the expectation values of the position and momentum operators ($\sigma_x = 0.5$, $\hbar = 1, m = 1$)

expansion can be used for the analytical potential functions in the studied domain. This series may not converge at finite number term truncations. Moreover, even if this series are convergent, the rate of the convergence may be very slow that causes increasing computational complexity of the presented method. In addition, there are some quantum mechanical systems which have potentials with singularities at finite argument values. Thus, it may be quite necessary to use Laurent series expansion. In that case, it is impossible to study directly with the position and the momentum operators. But, it is possible to study the function of these operators and to find the expectation values of those functions of operators such that the resulting value inverted by using the function under consideration if possible. The obtained entity may be called pseudo expectation values. This is under an intense study in the group of the second author. Another way to deal with this issue is to define a new "weighted expectation value" which can be explicitly given as follows.

$$\langle \widehat{o}(t) \rangle \equiv \int_{-\infty}^{\infty} dx \psi(x,t)^* w(x,t)^* o(t) w(x,t) \psi(x,t) \tag{61}$$

where $w(x,t)$ is the appropriately chosen weight function and satisfies the following property.

$$\int_{-\infty}^{\infty} dx \psi(x,t)^* w(x,t)^* w(x,t) \psi(x,t) = 1 \tag{62}$$

This approach can also be used to suppress both divergence of the series expansion of the potential function and to accelerate the convergence rate of the series expansion of the potential function. This topic is now under a detailed intense study via a PhD project conducted by Metin Demiralp.

Another way to deal with the aforementioned issue is to define a weighted system vector as follows.

$$\mathbf{s} \equiv \begin{bmatrix} w(H)pw(H) \\ w(H)qw(H) \end{bmatrix} \tag{63}$$

for the example system vector shown below

$$\mathbf{s} \equiv \begin{bmatrix} p \\ q \end{bmatrix} \tag{64}$$

using the fact that

$$\{H, w(H)\} = 0 \tag{65}$$

It can be quite necessary to truncate fluctuation expansion in large orders and this may lead divergence in the solution of the ODEs. This approach can be used to suppress this type of divergence due to the fact that momentum operator is unbounded. When this approach is used, the inverse transformation is needed to gather the knowledge of the desired expectation values of position and momentum operators. This inverse transformation may not always be well defined depending on the structure of the chosen weight function. Inspite of this drawback, it is still possible to extract physical information about the system under consideration from this type of pseudo expectation values.

Since, the approximation for the general type of potentials is very crucial for the presented method, the fluctuation expansion can be done around an optimized point. Moreover, different kinds of polynomial approximation schemes can also be considered. All these prospects can be considered as future studies even though some of them have recently been located to the loom (if the statement fits).

9 Conclusion

This study is the second part of the total framework which is called PEA to the quantum mechanical operators. The main focus of this study is to do quantum mechanics without explicitly solving Schrödinger equation but directly modeling the expectation values of the quantum mechanical operators. This is achieved conceptually in these papers.

While the first part of this couple of papers explores the Lie algebraic group closed in infinite dimension, this second part of the study introduces the mathematical theory of fluctuation expansion to be able to study the Lie algebraic group in finite dimension. The detailed discussion and related mathematical proof are given in this study. Also the theory is demonstrated with an example system, symmetric quartic anharmonic oscillator in one dimension composed of single particle. Some further developments of the theory is also discussed in this paper.

One of the most important further future direction is to explore the convergence properties of the method, when the studied operator space gets larger. As shown in the first paper, when this space is infinite only the asymptotic convergence is possible. Thus, the convergence is not guaranteed and even if it is obtained, it may or may not be uniform.

Another further future direction is to use this method to model the quantum mechanical effects such as tunneling and quantum zero point energy. The last but not the least, state to state or state to costate transition amplitudes appearing in the quantum optimal control theory is a candidate for the future application areas.

The method presented here is the one of the most strongest candidates of the studies about the correspondence between the classic and quantum mechanics. And, to the best of our knowledge, the method presented here is the most systemized approach due to the usage of Kronecker product and thus the easiest one to be implemented amongst the others.

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References

1. M. Ayvaz, M. Demiralp, Probabilistic evolution approach to the expectation value dynamics of quantum mechanical operators, part I:integral representation of Kronecker power series and multivariate Hausdorff moment problems, J. Math. Chem. (2014). doi:10.1007/s10910-014-0371-8
2. P. Ehrenfest, Bemerkungüber die angenäherte Gültigkeit der klassischen Mechanik innerhalb der Quantenmechanik. Z. Phys. **45**(7–8), 455–457 (1927)
3. M. Demiralp, No fluctuation approximation in any desired precision for univariate function matrix representations. J. Math. Chem. **47**, 99–110 (2010). doi:10.1007/s10910-009-9533-5
4. B. Tunga, M. Demiralp, Fluctuation free multivariate integration based logarithmic HDMR in multivariate function representation. J. Math. Chem. **49**, 894–909 (2012). doi:10.1007/s10910-010-9786-z
5. M. Demiralp, Various Parallel and Diversive Aspects of the Mathematical Fluctuations Theory with the Related Standing Issues, in 7th International Conference on Computational Methods in Science and Engineering (ICCMSE), AIP Conference Proceedings, vol. 1504, pp. 364–376 (2009). doi:10.1063/1.4771729
6. M. Ayvaz, M. Demiralp, A Fluctuation Analysis at the Classical Limit for the Expectation Dynamics of a Single Quartic Quantum Anharmonic Oscillator, in International Conference on Numerical Analysis and Applied Mathematics (ICNAAM), AIP Conference Proceedings, vol. 1281, pp. 1950–1953 (2010). doi:10.1063/1.3498311
7. M. Ayvaz, M. Demiralp, Quantum Optimal Control of Single Harmonic Oscillator Under Quadratic Controls together with Linear Dipole Polarizability: A Fluctuation Free Expectation Value Dynamical Perspective, in International Conference on Numerical Analysis and Applied Mathematics (ICNAAM), AIP Conference Proceedings, vol. 1389, pp. 364–376 (2011) doi:10.1063/1.3637828
8. M. Demiralp, E. Demiralp, L. Hernandez-Garcia, A probabilistic foundation for dynamical systems: theoretical background and mathematical formulation. J. Math. Chem. **58**, 850–869 (2012)
9. M. Demiralp, E. Demiralp, L. Hernandez-Garcia, A probabilistic foundation for dynamical systems: phenomenological reasoning and principal characteristics of probabilistic evolution. J. Math. Chem. **58**, 870–880 (2012)
10. M. Demiralp, E. Demiralp, A contemporary linear representation theory for ordinary differential equations: probabilistic evolutions and related approximants for unidimensional autonomous systems. J. Math. Chem. (2012). doi:10.1007/s10910-012-0070-2
11. M. Demiralp, E. Demiralp, A contemporary linear representation theory for ordinary differential equations: multilinear algebra in folded arrays (Folarrs) perspective and its use in multidimensional case. J. Math. Chem. (2012). doi:10.1007/s10910-012-0064-0
12. M. Demiralp, A probabilistic evolution approach trilogy, part 1: quantum expectation value evolutions, block triangularity and conicality, truncation approximants and their convergence, J. Math. Chem. (2012). doi:10.1007/s10910-012-0079-6
13. M. Demiralp, N.A. Baykara, A probabilistic evolution approach tri logy, part 2: spectral issues for block triangular evolution matrix, singularities, space extension, J. Math. Chem. (2012). doi:10.1007/s10910-012-0080-0

14. M. Demiralp, B. Tunga, A probabilistic evolution approach trilogy, part 3: temporal variation of state variable expectation values from Liouville equation perspective, J. Math. Chem. (2012) doi:10.1007/s10910-012-0081-z
15. C. Gozukirmizi, M. Demiralp, Probabilistic evolution approach for the solution of explicit autonomous ordinary differential equations, part 1: arbitrariness and equipartition theorem in Kronecker power series, J. Math. Chem. **51**(10) doi:10.1007/s10910-013-0298-5 (2013)
16. C. Gozukirmizi, M. Demiralp, Probabilistic evolution approach for the solution of explicit autonomous ordinary differential equations, part 2: kernel separability, space extension, and, series solution via telescopic matrices, J. Math. Chem. **51**(10) (2013). doi:10.1007/s10910-013-0299-4
17. O.V. Prezhdo, Y.V. Pereverzev, Quantized Hamilton dynamics. J. Chem. Phys. **113**(16), 6557–6565 (2000)
18. O.V. Prezhdo, Y.V. Pereverzev, Quantized Hamilton dynamics for a general potential. J. Chem. Phys. **116**(11), 4450–4461 (2002). doi:10.163/1.1451060
19. Y. Shigeta, H. Miyachi, K. Hirao, Quantal cumulant dynamics: general theory. J. Chem. Phys. **125**(24), 244102 (2006)