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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

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Abstract This is the first one of two companion papers focusing on the establishment of a new path for the expectation value dynamics of the quantum mechanical operators. The main goal of these studies is to do quantum mechanics without explicitly solving Schrödinger wave equation, in other words, without using wave functions except their initially given forms. This goal is achieved by using Ehrenfest theorem and utilizing probabilistic evolution approach (PEA). PEA, first introduced by Metin Demiralp, is a method providing solutions to the nonlinear ordinary differential equations by transforming them to a set of linear ODEs at the cost of denumerably infinite dimensionality. It is recently shown that this method produces analytic solutions, if the initial conditions are given appropriately at some special cases. However, generalization of these conditions to the quantum mechanical applications is not straightforward due to the dispersion of the quantum mechanical systems. For this purpose, multivariate moment problems for the integral representation of the Kronecker power series are introduced and then solved yielding to more specific and precise convergence analysis for the quantum mechanical applications.

Keywords Probabilistic evolution approach · Quantum mechanics · Expectation value dynamics · Hausdorff moment problem · Kronecker power series · Ordinary differential equations

Mathematics Subject Classification 15A18 · 34A05 · 34A12

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1 Introduction

The question of "Is it possible to model quantum mechanical phenomena without explicitly solving Schrödinger wave equation?" has been lying at the hearth of our and other researcher's studies during the last years. This question takes its importance from two aspects. The first one is the computational ineffectiveness of the Schrödinger equation because of multidimensionality especially when the system's degree of freedom increases unboundedly. The second and the most important aspect is to deepen the human kind's understandings of the quantum mechanical nature by establishing connections between quantum and the classical mechanics.

The computational expense to numerically solve Schrödinger equation becomes very high as the dimensionality of the system increases. Beyond that it may become impossible to get a reliable numerical solution even by using today's supercomputers. Considering quantum many body systems, the number of the freedom of the system under consideration may grow very rapidly in the coordinates and this situation makes it impossible to solve Schrdinger equation even with the aid of the modern computer architectures. Density Functional Theory, one of the seminal works related to answer that question and answering partly "yes" led to the Nobel Prize [1,2].[1] In last years, some variants of that theory such as Orbital Free Density Functional Theory developed [3–6]. All these approaches require solution of not the Schrödinger equation but the reduced number of other partial differential equations. Beside these leading research, Quantum Monte Carlo methods search for the answer and they all have the limited capability of calculating, even, ground state for the system under consideration.

In addition to the quantum many body systems, optimal control of the quantum phenomena requires computationally sophisticated algorithms due to the huge number of iterations and the necessity of solving Schrödinger equation up to a high degree of numerical accuracy. Since most of the numerical algorithms require or are based on discretization, the solution may fail to converge due to the error accumulations arising from discretization.

On the other hand, generally, the wave function is used for the determination of the expectation values and their time evolutions for certain entities such as position and momentum operators. The main philosophy of our research is to develop novel methodologies to be able to determine these expectation value dynamics utilizing Heisenberg equations of motion. Even though, the Heisenberg equations of motion are capable of defining dynamics of expectation values of certain quantum mechanical operators by ordinary differential equations, these equations fail to have a solution in the most of the cases due to the fact that the ODE defined for an operator involves at least one unknown expectation value of another operator which does not originally appear in the analysis. That is to say, the commutator algebra is closed under the Poisson bracket with the Hamiltonian, generally, only when it is studied for an infinite set of operators. Moreover, the set of ODEs gathered from Heisenberg equations of motion are generally nonlinear, depending on the system Hamiltonian, particularly

[1] Nobel Prize in chemistry in 1998. Interested reader may see Nobel lecture entitled "Electronic Structure of Matter—Wave Functions and Density Functionals" by Walter Kohn and references [1,2].

potential function. Thus, some brand new methodologies have to be developed to overcome this difficulty.

Probabilistic evolution approach (PEA) is a novel methodology developed to deal with the above mentioned issues. The main idea that lies at the hearth of this method can be summarized as follows. Every measurement contains certain level of uncertainty by principle, in natural sciences such as chemistry and physics related fields. This uncertainty can generally be characterized by using certain probability distribution functions. These may not be needed in some circumstances even if they may be always required by certain systems de pending on their structures. This probability distribution function appears to be Dirac delta function at the classical mechanics threshold (where the energy spectrum of a system is continuous by definition) of the quantum mechanics. However for the discrete spectrum involving cases of quantum dynamics and similar structures, it has to be defined within a sufficient precision because of the dispersive nature of the dynamics under consideration. This is usually provided by the solution of certain partial differential equations like Schrödinger equation. Quantum mechanical and statistical mechanical systems such as neuronal dynamics in neuroscience can be considered as examples of the discrete energy spectrum involving cases.

To fully describe system dynamics under consideration, it is usually necessary to determine how the expectation values of some operator entities, such as position and momentum in quantum mechanics, evolve forward or backward (or both) in time. This is achieved by determining and solving ordinary differential equations accompanied with some initial and/or boundary conditions. The general form of the solution of initial value problems is as follows:

$$\mathbf{x}(t) = \mathbf{P}(t)\mathbf{x}(0) \tag{1}$$

where $\mathbf{x}(0)$ denotes initial value and may be a vector entity while $\mathbf{P}(t)$, which has generally matrix or operator character, describes the time evolution of the system under consideration (it is generally called "Propagator").

Taking this main philosophy into account, PEA, determines the evolutionary entity, $\mathbf{P}(t)$, of the system numerically and analytically in certain cases. This is achieved by converting nonlinear ODEs to denumerably infinite set of linear homogeneous ODEs by using appropriate basis set expansions. The basis set is generally taken to be composed of power sets appearing in the Taylor series expansions. Fourier basis set is also used successfully to be able to model the systems whose behaviors are known to be periodic. PEA can also take the dispersion of the initial system entities into account by using a probabilistic moment generator for the initial impositions. If the probabilistic generator is in a Dirac delta function type structure then the initial values form a power set. Otherwise mathematical fluctuations are needed to relate them to power sets. The Mathematical Fluctuation Expansion Theory and its certain aspects will be discussed in a more detailed manner at the companion of this paper [7].

The main focus of this paper is to find a new form of the solutions of PEA for the quantum mechanical applications in such a way that it makes possible to clarify the conditions of convergent and analytic solutions. This is achieved by uniquely determining two different kinds finite interval moment problems: multivariate Hausdorff moment problem and matrix weighted Hausdorff moment problem.

After this brief introduction, the remaining part of the paper is organized as follows. Following section includes preliminary and general framework of the PEA. Definition of the three typical moment problems and their multivariate variants are given in the Sect. 3. The Sect. 4 includes the conditions for the existence and the explicitness of the solution to the multivariate Hausdorff moment problem while the Sect. 5 focuses on the extension of the fourth section to the cases where not the Kronecker powers but their images under an appropriately given square matrix valued function of the system vector are considered. The Sect. 6 discusses the utilization of square matrices whose types vary from element to element of the sequence at the focus. The paper will be finalized by giving certain further concluding comments and remarks to go to future directions as usual.

2 General framework of probabilistic evolution approach (PEA)

PEA is a recently proposed novel methodology which has the ability to convert (or truely speaking extend) a set of ODEs to a denumerably infinite set of linear and homogeneous ODEs first, and then, to produce approximate solutions to this infinite set of ODEs and to deal with nonlinearities and singularities in the potential function of the system under consideration up to some extend by utilizing Kronecker product and Kronecker powers [8–14]. The mathematical formulation of this method can be described concisely as follows. Without any loss of generality and for the sake of simplicity, the Hamiltonian of an isolated quantum mechanical system composed of a single particle moving on its line segment can be described as follows.

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

where $\widehat{p}$ and $\widehat{q}$ stand for the momentum and the position operators of the system under consideration, respectively. And, μ is the mass of the particle. We, here and hence forth, use the hat symbol to emphasize on operator nature. The Kronecker power series expansion of the potential function can be explicitly written as its Maclaurin series if there is only one degree of freedom for the system. For this case, Maclaurin series and the Kronecker power series match. In the systems with more than one degree of freedom, the potential function can be expressed in all nonnegative powers of the position operators and for conciseness we prefer to use the Kronecker power series which can be written as follows.

$$V(\widehat{q}) = \sum_{j=0}^{\infty} \mathbf{v}_j^T \widehat{\mathbf{r}}^{\otimes j} \tag{3}$$

where $\widehat{\mathbf{r}}$ stands for the vector whose components are the position operators each of which corresponds to a separate degree of freedom, and therefore, its dimensionality is the degree of freedom. In this equations, the linear combination coefficient, $\mathbf{v}_j$ stands for a vector of n^j elements where n denotes the system's degree of freedom. This dimensionality is because of the dimensionality balance of the equation in its both sides (as we are going to see soon, $\widehat{\mathbf{r}}$ is composed of n elements and enforces $\widehat{\mathbf{r}}^{\otimes j}$ to have n^j elements due to the definition of Kronecker power).

This structure can even be used for the univariate case when we attempt to use the "Space Extension" concept by regarding certain position operator dependent expressions as if they are independent entities. In such cases the vector $\widehat{\mathbf{r}}$'s elements are composed of linear and nonlinear functions of the position operator. Then, the abovementioned series expansion of the potential function can be obtained from the Maclaurin or Taylor series expansion if $V(\widehat{q})$ is analytic in the spectral domain of the position operators and $\widehat{r}$ contains positive integer powers of the position operator. If $V(\widehat{q})$ has polar singularities, the abovementioned series expansion can be obtained from Laurent series and, in that case, the vector $\widehat{\mathbf{r}}$ additionally or lonely contains negative powers of the position operators. In (3), "$\otimes$" and $(\cdot)^{\otimes j}$ denote the Kronecker product symbol and jth Kronecker power of a vector. Explicit structures are given as follows.

$$\mathbf{u} \otimes \mathbf{v} = \left[u_1 \mathbf{v}^T \;\; u_2 \mathbf{v}^T \;\; \ldots \;\; u_n \mathbf{v}^T \right]^T \tag{4}$$

$$\mathbf{u}^{\otimes j} = \mathbf{u} \otimes \mathbf{u}^{\otimes j-1}, \quad \mathbf{u}^{\otimes 0} = 1 \tag{5}$$

Beside all these definitions, so called "system vector" has to be defined to proceed. System vector is composed of momentum operator and previously defined vector $\widehat{r}$ as follows.

$$\mathbf{s} \equiv \left[\widehat{p} \; \widehat{\mathbf{r}}^T \right]^T \tag{6}$$

The expansion given in Eq. (3) is not unique in both coefficients and in the system vector definition, and therefore, has certain flexibilities. The dimension of the system vector depends on the choice of the vector $\widehat{\mathbf{r}}$ which may be generally specified after certain space extensions. The flexibilities mentioned above can be used for the algorithm development and analysis of PEA together with certain space extension strategies. These issues are considered beyond the scope of this work. After all these definitions, the time evolution of the system vector can be expressed as follows by using Ehrenfest theorem.

$$\frac{d\langle \mathbf{s} \rangle (t)}{dt} = \left\langle \frac{i}{\hbar} \left[\widehat{H}\mathbf{s} - \mathbf{s}\widehat{H} \right] \right\rangle \equiv \left\langle \left\{ \widehat{H}, \widehat{s} \right\} \right\rangle \tag{7}$$

where the rightmost representation is known as Poisson bracket. From (2), (3), and (6), it is not difficult to see that the following equality holds.

$$\left\{ \widehat{H}, \mathbf{s} \right\} \equiv \frac{i}{\hbar} \left[\widehat{H}\mathbf{s} - \mathbf{s}\widehat{H} \right] = \sum_{j=0}^{\infty} \mathbf{H}_j^{(p)} \mathbf{s}^{\otimes j} \tag{8}$$

where the superscript (p) is used to imply belonging to Poisson bracket. The coefficient entity, $\mathbf{H}_j^{(p)}$, except in the cases where $j = 0, 1$, is a rectangular matrix of $n \times n^j$

type. Now this is an operator algebraic equality. The right hand side expression's coefficient matrices except $\mathbf{H}_0^{(p)}$ and $\mathbf{H}_1^{(p)}$ involve uncertainties in their structures. These uncertainties can be characterized by certain number of parameters we call flexibilities. These flexibilities can be used to get certain properties in the set of coefficient matrices, like the convergence rate of their norms. A recent paper about these flexibilities proposes equipartition theorem dictating us to take the coefficients of same type multivariate terms equal in (8) [15,16]. After fixing the flexibilities in the rectangular matrix coefficients of (8), we get a unique equality over the given and therefore known entities, the Kronecker powers of the system vector of operators. Even though, these Kronecker powers are specified entities, their expectation values are unknown entities. The Ehrenfest theorem and (8) relates the time derivative of the system vector's expectation value to the Kronecker power expectation values of the system vector operator. These latter entities are also unknown and there is no direct way to relate them to the expectation value of the system vector operator through certain specified functions because of the probabilistic nature of the expectation values. All these urge us to establish an ODE for the jth Kronecker power of the system vector operator as follows.

$$\frac{d\left\langle \widehat{\mathbf{s}}^{\otimes j}\right\rangle(t)}{dt} = \left\langle \left\{ \widehat{H}, \mathbf{s}^{\otimes j} \right\} \right\rangle \tag{9}$$

Since it is very well-known that the Poisson bracket obeys Leibnitz rule of the product differentiation we can rewrite this equation as

$$\frac{d\left\langle \widehat{\mathbf{s}}^{\otimes j}\right\rangle(t)}{dt} = \left\langle \sum_{k=0}^{j-1} \mathbf{s}^{\otimes k} \otimes \left\{ \widehat{H}, \mathbf{s} \right\} \otimes \mathbf{s}^{\otimes j-k-1} \right\rangle \tag{10}$$

which can be combined with (8) and then the use of the fact that Kronecker product can be distributed over the matrix product (and vice versa) under the multiplicative consistency we can arrive at

$$\frac{d\left\langle \widehat{\mathbf{s}}^{\otimes j}\right\rangle(t)}{dt} = \sum_{k=0}^{\infty} \mathbf{E}_{j,k} \left\langle \widehat{\mathbf{s}}^{\otimes k}\right\rangle(t), \quad j = 1, 2, \ldots \tag{11}$$

where $\mathbf{E}_{j,k}$ is explicitly defined as follows.

$$\mathbf{E}_{j,m} \equiv \sum_{k=0}^{j-1} \left(\mathbf{I}_n^{\otimes k} \otimes \mathbf{H}_{m-j+1}^{(p)}(t) \otimes \mathbf{I}_n^{\otimes (j-k-1)} \right) \quad j, m = 0, 1, 2, 3 \ldots \tag{12}$$

As we have defined, the Evolution Matrix contains rectangular $\mathbf{E}_{j,k}$ matrices as its blocks and can be explicitly given as follows.

$$\mathbf{E} \equiv \begin{bmatrix} \mathbf{E}_{0,0} & \cdots & \mathbf{E}_{0,j} & \cdots \\ \vdots & \ddots & \vdots & \ddots \\ \mathbf{E}_{j,0} & \cdots & \mathbf{E}_{j,j} & \cdots \\ \vdots & \ddots & \vdots & \ddots \end{bmatrix} \tag{13}$$

After all these steps, countably many sets of linear ODEs can be obtained in the following form.

$$\frac{d\boldsymbol{\xi}(t)}{dt} = \mathbf{E}\boldsymbol{\xi}(t), \tag{14}$$

where,

$$\boldsymbol{\xi}(t) = \left[\left\langle \widehat{\mathbf{s}}^{\otimes 0} \right\rangle^T (t) \;\; \left\langle \widehat{\mathbf{s}}^{\otimes 1} \right\rangle^T (t) \;\; \ldots \right]^T \tag{15}$$

and the formal solution is as follows.

$$\boldsymbol{\xi}(t) = \mathrm{e}^{t\mathbf{E}} \boldsymbol{\xi}(0) \tag{16}$$

Since the evolution matrix is denumerably infinite, it is impossible to produce a practically utilizable solution from that equation unless somehow certain approximants (like truncation approximants) are defined. Thus, truncation approximants are perhaps best options to be employed. If the series expansion of the potential function given in (3) is finite, evolution matrix is not full but in block banded structure. To be able to produce solution from the above equation, the first step is to construct recurrence relations. This may bring us too much computational complexities both for the analysis and developing algorithms as long as the matrix $\mathbf{E}$ remains in full upper block Heisenberg form. Thus, it is necessary to construct evolution matrix in more eligible forms. This can be accomplished by adding a constant term and also adding some other nonlinear operator structures to the system vector. By these space extension strategies, it is possible to form evolution matrix in a banded structure of two adjacent block diagonals (one of which is the main block diagonal). Moreover, by constancy added space extension (CASE) temporal behavior can be removed (bringing autonomy) from the kernel of the resultant equation s of recurrence relations [8–16]. And formal final solution of the PEA can be written in the following form.

$$\langle \widehat{\mathbf{s}} \rangle (t) = e^{\beta t} \sum_{j=0}^{\infty} \frac{1}{j!} \left(\frac{e^{\beta t} - 1}{\beta} \right)^j \mathbf{T}_j \left\langle \mathbf{s}^{\otimes j+1} \right\rangle (0) \tag{17}$$

Computation of $\left\langle \mathbf{s}^{\otimes j+1} \right\rangle (0)$ requires the knowledge of the initial wave packet. Even though the initial wave packet is known, the task of computing $\mathbf{T}_j \left\langle \mathbf{s}^{\otimes j+1} \right\rangle (0)$ may be computationally expensive even if $\mathbf{T}_j$ is sparse due to the Kronecker product sum given in (12). On the other hand, these series are divergent everywhere on the studied domain except under certain conditions. The necessary conditions were mentioned in some previous studies [12]. Thus, it is a very important task to clarify sufficient conditions for the convergence or to extract knowledge from these divergent series. For this purpose, it is necessary to write these series in another form as follows.

$$\langle \widehat{\mathbf{s}} \rangle (t) = \int_V dV W(\mathbf{x}) e^{\beta t} \sum_{j=0}^{\infty} \frac{1}{j!} \left(\frac{e^{\beta t} - 1}{\beta} \right)^j \mathbf{T}_j \mathbf{x}^{\otimes j} \tag{18}$$

Another form can be considered as follows.

$$\langle \widehat{\mathbf{s}} \rangle (t) = \int_V dV e^{\beta t} \sum_{j=0}^{\infty} \frac{1}{j!} \left(\frac{e^{\beta t} - 1}{\beta} \right)^j \mathbf{T}_j \mathbf{W}_j(\mathbf{x}) \mathbf{x}^{\otimes j} \tag{19}$$

These are more eligible forms to reduce the computational complexity because of the direct usage of the Kronecker powers of vectors and also some algorithms currently developed for this purpose. To achieve this, our first approach is to define a multivariate finite interval Hausdorff moment problem.

3 Definition of the multivariate moment problem

The univariate moment problem is defined as seeking an inverse mapping from a given sequence to its related measure. More concisely it can be defined as follows.

$$\mu_j \equiv \int_a^b dx W(x) x^j, \quad j = 0, 1, 2, \ldots \tag{20}$$

where the symbol $W(x)$ characterizes an unknown function which can be considered as generating function even though it is expected to be a true weight function. μ_j stands for the given sequence elements (these are called "moments" if the generating function $W(x)$ becomes a true weight function). Typically, there are three kinds of moment problems. These are, (1) Hausdorff moment problem in which the interval is considered to be bounded; (2) Stieltjes moment problem which is corresponding to a semi-infinite interval; and, (3) Hamburger moment problem defined over the fully infinite interval.

In this study we will go beyond the univariance and consider the multivariate Hausdorff moment problem, via Kronecker power sequences defined as follows.

$$\boldsymbol{\mu}_j \equiv \int_V dV W(\mathbf{x}) \mathbf{x}^{\otimes j}, \quad j = 0, 1, 2, \ldots \tag{21}$$

where $\boldsymbol{\mu}_j$ corresponds to jth element of the sequence at the focus. It is a vector whose dimensionality changes from j value to j value.[2] $\mathbf{x}$ stands for an n-element vector and may be called "System vector" due to inspiration from dynamical systems. The Kronecker power definition of the previous sections remains also valid here. $W(\mathbf{x})$ stands for a generating function we desire to prove that it becomes a weight function under the satisfaction of certain conditions. In this formula, V denotes a finite rectangular hyperprism positioned in a finite region of the Cartesian space spanned by the elements of the vector $\mathbf{x}$ such that its each edge is parallel to a separate coordinate axis. Whereas dV denotes the volume element in this n-dimensional Cartesian space.

In univariate case the interval of Hausdorff moment problem is finite but it can always be converted to the standard unit interval $[\,0, 1\,]$ through an appropriate affine transformation. Same thing can also be done here, in the multivariate case, and the abovementioned hyperprism can be converted to a unit hypercube whose one corner is located at the origin while each of the others resides on a different positive coordinate axis. Even though this standardization may gain importance for practicality we do not really need it in this conceptual analysis.

All these imply that $\boldsymbol{\mu}_j$ has n^j components. In other words, the sequence under consideration is constructed by elements with different and increasing dimensionalities (this is some how out of our familiarities but is required to use Kronecker powers here).

In the sense of quantum dynamics under PEA, $\boldsymbol{\mu}_j$s correspond to $\left\langle \mathbf{s}^{\otimes j} \right\rangle (0)$s. Since this latter entity may become very dispersive as j grows, depending on the initial wave function and the system under consideration, PEA solutions may become only asymptotically converging. Hence, expressing them via moment-like-integrals may bring uniform convergence to their integral representation kernels that urges us to use Borel sum techniques to get sums of divergent series. This is the reason why we spend so much effort for the investigations of these types issues here.

The definition and the solution of multivariate finite region Hausdorff moment problem of this type is a novel issue even though certain results have been reported [17, 18] by using multivariate Taylor series structures. The use of Kronecker power series somehow condensates the results of multiindex formulation involving theories. Hence, we can state that the main contribution of this study is both in the research area of moment problem and of PEA within Kronecker power series perspective.

The abovementioned multivariate moment problem can be extended to the investigation of the sequences over the following elements

$$\boldsymbol{\mu}_j \equiv \int_V dV w(\mathbf{x}) \left[\, \mathbf{W}(\mathbf{x})\, \mathbf{x} \,\right]^{\otimes j}, \quad j = 0, 1, 2, \ldots \tag{22}$$

[2] At this point it is better to emphasize on how the mathematical object "Sequence" is defined. It is known as "A list of elements". It is not a set because the repetition of the elements is allowed and, beyond that, the elements should be ordered. The general tendency is to use same type elements, that is, the objects sharing at least one property like in positive integers, rational numbers, and so on. Here, the shared property is the global definition, "the integral of a given so-called state vector's Kronecker powers under a generating function factor".

where everything is same as before except the new entity $\mathbf{W}(\mathbf{x})$ which is an $n \times n$ type matrix valued function of the system vector. $\mathbf{W}(\mathbf{x})$ is introduced to reflect the interaction between the elements of the system vector. Our anticipation is that the introduction of this entity may bring certain flexibilities to the practical determination of the function $w(\mathbf{x})$. This issue is focused on in the fifth section.

Another moment-like problem considered in this study uses a matrix generating function which appears in place of the weight function of the above analysis. We focus on the following sequence elements generated over the Kronecker powers of the so-called system vector $\mathbf{x}$

$$\boldsymbol{\mu}_j \equiv \int_V dV \mathbf{W}_j(\mathbf{x})\, \mathbf{x}^{\otimes j}, \quad j = 0, 1, 2, \ldots \tag{23}$$

where $\boldsymbol{\mu}_j$ stands for the same thing as we mentioned above and may be correspondant to $\left\langle \mathbf{s}^{\otimes j} \right\rangle (0)$ in PEA for the quantum dynamical evolution. In contrast to the above cases, $\mathbf{W}_j(\mathbf{x})$ is a matrix valued unknown generating function we desire to get it as a matrix valued weight function. The j dependence in this matrix is mandatory because of the need for the multiplicative consistency at the right hand side kernel. In this type problems the entities to be determined are infinitely many because of j dependence. This brings the possibility of creating an infinite set of matrix valued functions which may be called generating function basis. We focus on this type problems in the sixth section.

Our basic intention to deal with this type of generating function problem is for enabling the model the dependencies between the expectation values of different operators included in the Kronecker powers of the system vector under the abundance of generating function basis functions. We expect somehow to characterize inter-operator interactions.

We restrict ourselves with the finite region moment problem, even though the Stieltjes moment problem can also be considered and solved in a way similar to the one presented in this paper. The comparison of these moment problem solutions' efficiency is left as a future work and considered beyond the scope of this study.

4 Solution of multivariate Hausdorff moment problem

4.1 Positive definiteness of the multivariate case Hankel matrices

In his pioneering works, Felix Hausdorff stated that Hausdorff moment problem for the univariate case has a unique solution if the Hankel matrices of all types for the problem are positive definite [19,20]. The same property exists for the multivariate case. The Extended Hankel matrices[3] can be defined in block structure for multivariate case as follows.

$$\mathbf{H}_m \equiv \begin{bmatrix} \mathbf{M}_{0,0} & \mathbf{M}_{0,1} & \dots & \dots \\ \mathbf{M}_{1,0} & \mathbf{M}_{1,1} & \dots & \dots \\ \dots & \dots & \ddots & \dots \\ \dots & \dots & \dots & \mathbf{M}_{m,m} \end{bmatrix} \tag{24}$$

where

$$\mathbf{M}_{j,k} \equiv \int_V dV W(\mathbf{x}) \mathbf{x}^{\otimes j} \mathbf{x}^{\otimes k^T}, \qquad j, k = 0, 1, 2, \dots, m \tag{25}$$

and therefore, $\mathbf{M}_{j,k}$ is a matrix of $n^j \times n^k$ type when we use an $\mathbf{x}$ vector composed of n elements. If this Extended Hankel matrix is positive definite, it must satisfy the following property for any $(1 + n + n^2 + \cdots + n^m)$-element vector $\mathbf{y}$.

$$q(\mathbf{y}) \equiv \mathbf{y}^\dagger \mathbf{H}_m \mathbf{y} > 0 \tag{26}$$

where the symbol † stands for the Hermitian conjugation (even though we may not need the complex valuedness here, we have desired the warranty of the validity for the extensions to the complex valuedness).

Using (25) in (26) implies

$$\begin{aligned} q(\mathbf{y}) &= \sum_{j,k}^{m} \mathbf{y}_j^\dagger \mathbf{M}_{j,k} \mathbf{y}_k \\ &= \int_V dV W(\mathbf{x}) \left[\sum_{j=0}^{m} \mathbf{y}_j^\dagger \mathbf{x}^{\otimes j} \right] \left[\sum_{k=0}^{m} \mathbf{x}^{\otimes k^T} \mathbf{y}_k \right] \\ q(\mathbf{y}) &= \int_V dV W(\mathbf{x}) \left| \phi(\mathbf{x}, \mathbf{y}) \right|^2 \end{aligned} \tag{27}$$

where | | is used to symbolize complex modulus and the scalar function $\phi(\mathbf{x}, \mathbf{y})$ is defined as

$$\phi(\mathbf{x}, \mathbf{y}) = \sum_{k=0}^{m} \mathbf{x}^{\otimes k^T} \mathbf{y}_k \tag{28}$$

[3] The true definition of Hankel matrices requires the equivalence of all elements in its each anti-diagonal. It is satisfied if the matrix $\mathbf{x}$ becomes a one-element vector, mainly scalar. The multivariance destroys the equivalence amongst the antidiagonal elements. However, we still keep the word “Hankel” in this matrix to recall the inspirations from the Hankel matrices even though we somehow emphasize on the discrimination by using the word “Extended” in the name of present case matrices.

and, beyond that, $\mathbf{y}_j$ is the jth subvector of $\mathbf{y}$. Now all these imply that $q(\mathbf{y})$ becomes positive as long as $W(x)$ remains nonnegative and $\phi(\mathbf{x}, \mathbf{y})$ does not identically vanish for some nonzero $\mathbf{y}$ vectors. The Kronecker powers, except the zeroth and first one, of the vector $\mathbf{x}$ which is assumed to be composed of linearly in dependent elements, have in fact linearly dependent elements. This can be easily noticed as follows: (1) The zeroth Kronecker power of $\mathbf{x}$ is just the scalar 1 by convention while the first Kronecker power of $\mathbf{x}$ is composed of linearly independent elements; (2) The second Kronecker power of $\mathbf{x}$ involves the squares of its elements and all possible binary products of those elements. The squares are single while each binary product appears twice, like x_1x_2 and x_2x_1 which are identical because of commutativity; (3) The number of terms which repeatedly appear as the elements of the higher Kronecker powers of $\mathbf{x}$ increases very rapidly as the Kronecker power grows.

For example, in the case where $\mathbf{x}$ is composed of just two elements, x_1 and x_2; the elements of the second Kronecker power of $\mathbf{x}$ are respectively $x_1^2,\ x_1x_2,\ x_2x_1$ and x_2^2. Certainly there is a repetition and $\mathbf{x}^{\otimes 2}$ has not 4 but 3 linearly independent elements, say $x_1^2,\ x_1x_2$, and, x_2^2. This situation is reflected to the $\mathbf{x}^{\otimes 2}$ involving portion of $\phi(\mathbf{x}, \mathbf{y})$ as follows

$$\mathbf{x}^{\otimes 2^T}\mathbf{y}_2 = y_1^{(2)}x_1^2 + \left(y_2^{(2)} + y_3^{(2)}\right)x_1x_2 + y_4^{(2)}x_2^2. \tag{29}$$

where "y"s superscripted by (2) are the elements of the vector $\mathbf{y}_2$. This expression can identically vanish when $\mathbf{y}_2$ becomes proportional to the vector $[\,0, 1, -1, 0\,]^T$ where the proportionality factor needs not to vanish. In other words, this expression can vanish for certain nonzero $\mathbf{y}_2$ values. Truely speaking, it vanishes when $\mathbf{y}_2$ resides on the straight line spanned by the vector $[\,0, 1, -1, 0\,]^T$ in four dimensional Cartesian space. If we consider a $\mathbf{y}$ vector whose all subvectors, except $\mathbf{y}_2$ which resides on the straight line spanned by the vector $[\,0, 1, -1, 0\,]^T$ in four dimensional Cartesian space, vanish then that $\mathbf{y}$, which is certainly nonzero, sets the value of the scalar function $\phi(\mathbf{x}, \mathbf{y})$ equal to zero. This takes us to the conclusion that $q(\mathbf{y})$ vanishes at least for this nonzero $\mathbf{y}$ vector.

Certain similar circumstances can be encountered for the terms involving higher Kronecker powers of $\mathbf{x}$. In those cases, more than one vectors orthogonal to the focused Kronecker power of $\mathbf{x}$ can be defined and all corresponding $\mathbf{y}$ subvectors residing on anyone of the lines spanned by these vectors annihilate the corresponding terms in $\phi(\mathbf{x}, \mathbf{y})$. All these analyses dictate us that there are some nonzero $\mathbf{y}$ vectors setting $\phi(\mathbf{x}, \mathbf{y})$ identically equal to zero. Evidently, $q(\mathbf{y})$ vanishes for those $\mathbf{y}$ vectors while it remains positive for all other $\mathbf{y}$ vector values as long as $W(\mathbf{x})$ is a true weight function.

The above discussions and progresses can be considered as the proof of the following theorem:

Theorem 1 *If $W(\mathbf{x})$ symbolizes a true weight function then the multivariate case Extended Hankel Matrix $\mathbf{H}_m$ is positive definite for $m = 0$ and $m = 1$ while it is at least positive semi-definite when $m \geq 2$ over the $\left(1 + n + n^2 + \cdots + n^m\right)$-dimensional Cartesian space.*

The statement of this theorem is not somehow what we have expected. Our expectation was not the semi-definiteness but definiteness. This semi-definiteness is in fact because of the existence of zero eigenvalues and corresponding eigenvectors. We somehow need to get rid of them. To this end we can again consider the quite simple case where $\mathbf{x}$ is composed of the elements, x_1 and x_2. The coefficient vector for $\mathbf{x}^{\otimes 2}$ is $\mathbf{y}_2$ which is composed of $y_1^{(2)}$, $y_2^{(2)}$, $y_3^{(2)}$, $y_4^{(2)}$ elements. If we use the equipartition theorem which has been quite recently conjectured and proven [15,16] then we have to take $y_2^{(2)} = y_3^{(2)}$. This is certainly a restriction over the four dimensional Cartesian space where $\mathbf{y}_2$ lies. This restriction corresponds to another restriction over the vector $\mathbf{y}$ in a greater dimensional space. Since the restriction equation is linear and homogeneous (otherwise not subspace but maybe a manifold is obtained), the vectors obeying this restriction span a subspace in a dimensionality one less than the dimension of original space where $\mathbf{y}$ lies. We may denote this restriction by the superscript (res) when we need to distinguish the related entities from the others.

The restriction is not peculiar to $\mathbf{y}_2$ and to the cases where $n = 2$. All the other cases and related vectors except $\mathbf{y}_0$ and $\mathbf{y}_1$ have restrictions and dimension reduction s to form subspaces. We call the subspace of $(1 + n + \cdots + n^m)$-dimensional Cartesian space which is spanned by the $\mathbf{y}^{(res)}$ vectors whose subvectors are accordingly and fully (all possible restrictions coming from the equipartition theorem are considered) restricted, "Equipartition Based Restriction Space" for the $(1 + n + \cdots + n^m)$-dimensional Cartesian space. As long as we consider quadratic form over this Restriction Space, it is possible to show that the function $\phi(\mathbf{x}, \mathbf{y})$ never identically vanishes for nonzero restricted $\mathbf{y}^{(res)}$ vectors (or "over the Restriction Space"). This urges us to conjecture the following theorem whose proof can be easily given by using these ideas here even though we do not intend to give the details.

Theorem 2 *If* $W(\mathbf{x})$ *symbolizes a true weight function then the multivariate case Extended Hankel Matrix* $\mathbf{H}_m$ *is positive definite for all nonnegative integer m values over the Equipartition Theorem Based Restriction Space of the* $(1+n+n^2+\cdots+n^m)$*-dimensional Cartesian space.*

The positive definiteness of $\mathbf{H}_m$ implies that its all up per leftmost square truncations are also positive definite on the Equipartition Theorem Based Restriction Space. These theorems guarantee the positive definiteness of the multivariate case Hankel matrices only when $W(\mathbf{x})$ stands for a true weight function. Otherwise, positive definiteness and positive semi-definiteness can not survive for all m values. This takes us to the following theorems which are in fact reverses of Theorems 1 and 2.

Theorem 3 *If all of the multivariate case Extended Hankel Matrices,* $\mathbf{H}_m$*s are positive definite for* $m = 0, 1$ *and semi-definite for* $m \geq 2$ *over the* $(1 + n + n^2 + \cdots + n^m)$*-dimensional Cartesian space then the function* $W(\mathbf{x})$ *becomes a true weight function (however it may vanish on a finite number subspace with a dimensionality less than the dimension of the original space under consideration).*

Theorem 4 *If all of the multivariate case Extended Hankel Matrices,* $\mathbf{H}_m$*s, are positive definite for all nonnegative integer m values over the Equipartition Theorem Based Restriction Space of the* $\left(1 + n + n^2 + \cdots + n^m\right)$*-dimensional Cartesian space then the function* $W(\mathbf{x})$ *is positive definite (is a weight function which is always positive).*

The last two theorems are about the existence of a true weight function for the $\boldsymbol{\mu}_j$s. This weight function becomes determinate (can be uniquely determined) in the case of the positive definiteness as we are going to show in the next subsection.

4.2 Determining the weight function

Let us now use a weight function $\Omega(\mathbf{x})$ whose explicit structure is known by us, and, consider the following function

$$f(\mathbf{x}) \equiv \frac{W(\mathbf{x})}{\Omega(\mathbf{x})} \tag{30}$$

whose utilization in (21) converts the multivariate case moment problem to the following form

$$\boldsymbol{\mu}_j \equiv \int_V dV \Omega(\mathbf{x}) f(\mathbf{x}) \mathbf{x}^{\otimes j}, \quad j = 0, 1, 2, \ldots \tag{31}$$

We may assume that the function f can be expanded to the following Kronecker power series

$$f(\mathbf{x}) = \sum_{k=0}^{\infty} \mathbf{f}_k^T \mathbf{x}^{\otimes k} \tag{32}$$

where $\mathbf{f}_k$ stands a vector of n^k elements which can be evaluated by using the known structure of the function f. This expansion urges us to write

$$\begin{aligned} \boldsymbol{\mu}_j &= \sum_{k=0}^{\infty} \int_V dV \Omega(x) \mathbf{f}_k^T \mathbf{x}^{\otimes k} \otimes \left(\mathbf{I}_{n^j} \mathbf{x}^{\otimes j}\right) \\ &= \sum_{k=0}^{\infty} \left(\mathbf{f}_k^T \otimes \mathbf{I}_{n^j}\right) \int_V dV \Omega(\mathbf{x}) \mathbf{x}^{\otimes k+j} \end{aligned} \tag{33}$$

where $\mathbf{I}_{n^j}$ denotes $n^j \times n^j$ type identity matrix and we have used the fact that a Kronecker product can be distributed over the matrix product and vice versa as long as the multiplicative consistency is protected amongst the factors. The symbolization of the rightmost integral on the right hand side of the above equation by $\boldsymbol{\omega}_{k+j}$, that is,

$$\boldsymbol{\omega}_{k+j} \equiv \int_V dV \Omega(\mathbf{x}) \mathbf{x}^{\otimes k+j}, \tag{34}$$

enables us to get

$$\boldsymbol{\mu}_j = \sum_{k=0}^{\infty} (\mathbf{f}_k^T \otimes \mathbf{I}_{n^j}) \boldsymbol{\omega}_{k+j}, \quad j = 0, 1, \ldots \tag{35}$$

To proceed we need to define

$$\mathbf{R}_{k,j}^{(\Omega)} = \left[\mathbf{m}_1 \quad \mathbf{m}_2 \quad \ldots \quad \mathbf{m}_{n^k} \right] \tag{36}$$

where $\mathbf{m}_i$ is the $n^j \times 1$ dimensional subvector of the vector $\boldsymbol{\omega}_{k+j}$ and $\mathbf{R}_{k,j}^{(\Omega)}$ is an $n^j \times n^k$ type matrix. This procedure may be called "folding procedure" because of its nature. Using this definition together with the following Kronecker product property amongts three multiplicatively consistent matrices, $\mathbf{A}$, $\mathbf{B}$, $\mathbf{Y}$

$$(\mathbf{B}^T \otimes \mathbf{A}) \text{vec}(\mathbf{Y}) = \text{vec}(\mathbf{AYB}) \tag{37}$$

where vec symbolizes an operator that produces a vector from a given matrix by the "unfolding procedure".

All these permit us to write

$$\begin{aligned} \left(\mathbf{f}_k^T \otimes \mathbf{I}_{n^j}\right) \boldsymbol{\omega}_{k+j} &= \left(\mathbf{f}_k^T \otimes \mathbf{I}_{n^j}\right) \text{vec}\left(\mathbf{R}_{k,j}^{(\Omega)}\right) \\ &= \text{vec}\left(\mathbf{I}_{n^j} \mathbf{R}_{k,j}^{(\Omega)} \mathbf{f}_k\right) \\ &= \mathbf{R}_{k,j}^{(\Omega)} \mathbf{f}_k \end{aligned} \tag{38}$$

The utilization of this equality in (27) produces the following linear system of equations

$$\boldsymbol{\mu}_j = \sum_{k=0}^{\infty} \mathbf{R}_{k,j}^{(\Omega)} \mathbf{f}_k, \quad j = 0, 1, 2, \ldots \tag{39}$$

where, as can be shown without any remarkable difficulty,

$$\mathbf{R}_{k,j}^{(\Omega)} \equiv \int_V dV \Omega\left(\mathbf{x}\right) \mathbf{x}^{\otimes j} \mathbf{x}^{\otimes k^T}, \qquad j, k = 0, 1, 2, \ldots \tag{40}$$

which means that the blocks of $\boldsymbol{\mathcal{R}}$ are the blocks of multivariate case Extended Hankel Matrices for the weight function $\Omega\left(\mathbf{x}\right)$. This fact makes the denumerably infinite coefficient matrix in (39) positive definite over the Equipartition Theorem Base Restriction Space we have previously defined.

The equations in (39) can also be written in the following matrix form

$$\boldsymbol{\mathcal{R}}_{\infty} \mathbf{f}_{\infty} = \boldsymbol{\mu}_{\infty} \tag{41}$$

where

$$\mathbf{f}_{\infty} \equiv \begin{bmatrix} \mathbf{f}_0 \\ \mathbf{f}_1 \\ \vdots \\ \vdots \end{bmatrix}, \quad \boldsymbol{\mu}_{\infty} \equiv \begin{bmatrix} \boldsymbol{\mu}_0 \\ \boldsymbol{\mu}_1 \\ \vdots \\ \vdots \end{bmatrix} \tag{42}$$

and

$$\mathcal{R}_{\infty} \equiv \begin{bmatrix} \mathbf{R}_{0,0}^{(\Omega)} & \mathbf{R}_{0,1}^{(\Omega)} & \cdots \\ \mathbf{R}_{1,0}^{(\Omega)} & \mathbf{R}_{1,1}^{(\Omega)} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}. \tag{43}$$

Thus, the solution of the finite interval moment problem can be obtained from the solution of a denumerably infinite linear algebraic equation system given by (39). The denumerably infinite coefficient matrix of this equation is positive semi definite as we have investigated before (just replacing W by Ω takes us to this judgement). The semi-definitiness imply the existence of zero eigenvalues and therefore the nullspace of the coefficient matrix in (39) is not empty. This may break the solvability of the equations in (39). However it is not hard to show that the right hand side infinite vector of (39) is orthogonal to the null space of the coefficient matrix of the same equation. This is because of the Kronecker power structure in the definition of the right hand side vector. In fact the vectors spanning the null space of the co efficient matrix of this equations are defined as being orthogonal to the Kronecker powers of the vector $\mathbf{x}$ such that the orthogonality remains valid without being affected from the values of the vector $\mathbf{x}$. This orthogonality between the right hand side vector and the left hand side coefficient matrix nullspace guarantees the solvability of the equations in (39). Despite this solvability we may not obtain uniqueness because of the appearance of an arbitrary infinite linear combination of the nullspace spanning vectors of this equation in the solution. On the other hand these arbitrarinesses disappear when they are plugged in the related places in the Kronecker power representation of the function $f(\mathbf{x})$. Hence all the coefficients in the arbitrary linear coefficients can be taken equal to zero without any loss of generality. This brings the uniqueness. All this discussions can be gathered in the following statement: "The solution of (41) over the Equipartition Theorem Based Restriction Space is unique".

Since we have chosen $\Omega(\mathbf{x})$ as a weight function, it can vanish only a finite number of at most $(n-1)$-dimensional subregion of n-dimensional Cartesian space. However its selection is at our disposal and it resides in the denominator of the f's definition. To avoid singularities it is better to choose this auxiliary weight function positive everywhere in the integration domain. This guarantees a nonvanishing nature in the integration domain for the function f. Thus, the unique determination of the function f can be reflected to the function W for the uniqueness in W determination. This completes the analysis for the weight function determination and urges us to write the following theorem.

Theorem 5 *If the multivariate case Extended Hankel Matrices* $\mathbf{H}_m$*s are all positive definite over the corresponding Equipartition The orem Based Restriction Spaces then the weight function* $W(\mathbf{x})$ *can be uniquely determined for the given* $\boldsymbol{\mu}_j$ *vectors. And then the set of these vectors can be called "Multivariate Kronecker Power Moment Sequence".*

The direct solution of (41) is impossible due to infinity in the structure unless certain very specific situations are under consideration. However, it is possible to truncate this equation to finite linear algebraic equations and then to get approximants whose qualities increase as the truncation order is taken to infinity. The convergence can be investigated through the utilization of the escalator method. We do not intend to get in to the details of this practical and technical issue.

5 Multivariate case extended Hausdorff moment problem over the images of system vector under a matrix transformation

In this case the sequence elements are defined as follows

$$\boldsymbol{\mu}_j \equiv \int_V dV w(\mathbf{x}) \left[\mathbf{W}(\mathbf{x}) \mathbf{x} \right]^{\otimes j}, \quad j = 0, 1, 2, \ldots \tag{44}$$

where the previously used scalar $W(\mathbf{x})$ function is denoted by $w(\mathbf{x})$ while the system vector is replaced with its image under the transformation by a square matrix of $n \times n$ type, denoted as $\mathbf{W}(\mathbf{x})$.

The so-called Extended Hankel Matrix is defined via the following formula as before

$$\mathbf{H}_m \equiv \begin{bmatrix} \mathbf{M}_{0,0} & \mathbf{M}_{0,1} & \ldots & \ldots \\ \mathbf{M}_{1,0} & \mathbf{M}_{1,1} & \ldots & \ldots \\ & & \ddots & \\ \ldots & \ldots & & \ldots \\ \ldots & \ldots & \ldots & \mathbf{M}_{m,m} \end{bmatrix} \tag{45}$$

while, now,

$$\mathbf{M}_{j,k} \equiv \int_V dV w(\mathbf{x}) \left[\mathbf{W}(\mathbf{x}) \mathbf{x} \right]^{\otimes j} \left[\mathbf{W}(\mathbf{x}) \mathbf{x} \right]^{\otimes k^T}, \qquad j, k = 0, 1, 2, \ldots, m \tag{46}$$

The previously defined scalar function $\phi(\mathbf{x}, \mathbf{y})$ takes the following new form

$$\phi(\mathbf{x}, \mathbf{y}) = \sum_{k=0}^{m} \left[\mathbf{W}(\mathbf{x}) \mathbf{x} \right]^{\otimes k^T} \mathbf{y}_k \tag{47}$$

This information is sufficient for repeating the analysis in the previous section for this case. Even though we do not intend to explicitly give the intermediate steps, it is possible to conjecture theorems 1–4, revised for this case, and then prove. Only new thing is the matrix valued function $\mathbf{W}(\mathbf{x})$ and as long as it is nonsingular there is no change in the previously done brainstorming. However, its nonempty nullspace affects almost everything to get the new theorems and proofs. Since $\mathbf{W}(\mathbf{x})$ is at our disposal we may assume its nonsingularity and avoid possible complications which may bring singularities. In fact nonsingularity can be considered not so much great restriction for the practicality. Hence we suffice with the nonsingular cases here.

The conjecture and the proof of the Theorem 5 can be realized for its revised form for this case. However, in this case, we need to write, first,

$$f(\mathbf{x}) \equiv \frac{W(\mathbf{x})}{\Omega(\mathbf{x})} \tag{48}$$

where $\Omega(\mathbf{x})$ stands for a known function as we assumed previously. This takes us to the following formula

$$\boldsymbol{\mu}_j \equiv \int_V dV \Omega(\mathbf{x}) f(\mathbf{x}) \left[\mathbf{W}(\mathbf{x}) \mathbf{x} \right]^{\otimes j}, \quad j = 0, 1, 2, \ldots \tag{49}$$

where we are going to prefer to use the following Kronecker power series not over the system vector but over its image under the mapping realized by using $\mathbf{W}(\mathbf{x})$

$$f(\mathbf{x}) = \sum_{k=0}^{\infty} \mathbf{f}_k^T \left[\mathbf{W}(\mathbf{x}) \mathbf{x} \right].^{\otimes k} \tag{50}$$

The analysis to get the expansion coefficients here is almost exactly same as before and takes us to the same conclusions as long as the matrix $\mathbf{W}(\mathbf{x})$ is nonsingular. We find this analysis for this case sufficient within the goal of this work.

6 Sequences via integrals over weighted Kronecker powers

We are going to consider the sequence whose elements are defined as follows in this section

$$\boldsymbol{\mu}_j \equiv \int_V dV \mathbf{W}_j(\mathbf{x}) \mathbf{x}^{\otimes j}, \quad j = 0, 1, 2, \ldots \tag{51}$$

which is somehow extended form of the sequence elements dealt with in the previous section. Indeed, the selection of the following expression

$$\mathbf{W}_j(\mathbf{x}) \equiv w(\mathbf{x}) \mathbf{W}(\mathbf{x})^{\otimes j}, \qquad j = 0, 1, 2, \ldots \tag{52}$$

takes us to the case of the previous section. This expression is however dependent on two entities: a common scalar function w and the matrix $\mathbf{W}$. These entities can be however considered as the generators of the $\mathbf{W}_j$ matrix valued weight functions. Here we extend the situation to somehow denumerable infinitely many generators, $\mathbf{W}_j$s' themselves.

Here we are not going to start the analysis by defining Extended Hankel Matrices as we did in the last two sections. Instead we are going to try to find a way for the evaluation of the matrix $\mathbf{W}_j(\mathbf{x})$ rather easily. To this end, we may be inspired from (52) and, as a first step, write

$$\mathbf{W}_j(\mathbf{x}) \equiv \omega(\mathbf{x})\,\mathbf{F}_j(\mathbf{x})\,\boldsymbol{\Omega}(\mathbf{x})^{\otimes j}, \qquad j = 0, 1, 2, \ldots \tag{53}$$

which replaces 51 with the following equation

$$\boldsymbol{\mu}_j \equiv \int_V dV \omega(\mathbf{x})\,\mathbf{F}_j(\mathbf{x})\,[\,\boldsymbol{\Omega}(\mathbf{x})\,\mathbf{x}\,]^{\otimes j}, \quad j = 0, 1, 2, \ldots \tag{54}$$

where apparently

$$\mathbf{F}_j(\mathbf{x}) = \frac{1}{\omega(\mathbf{x})}\mathbf{W}_j(\mathbf{x})\left[\,\boldsymbol{\Omega}(\mathbf{x})^{\otimes j}\,\right]^{-1} \tag{55}$$

which implies that we need the invertability of the scalar $\omega(\mathbf{x})$ and the matrix $\boldsymbol{\Omega}(\mathbf{x})$. This is always possible since the choice of $\omega(\mathbf{x})$ and $\boldsymbol{\Omega}(\mathbf{x})$ is at our disposal. To facilitate the further analysis we are going to prefer to work with the true weight function type entities and we assume that $\omega(\mathbf{x})$ and $\boldsymbol{\Omega}(\mathbf{x})$ are positive everywhere in the integration domain. This assumption enables us to expand $\mathbf{F}_j(\mathbf{x})$ to a Kronecker power series. However, here we do not use the Kronecker powers of the system vector. Instead, we deal with the Kronecker powers of the system vector' s image under an appropriately chosen square matrix valued function of system vector.

Before proceeding we can again focus on (54) where $\boldsymbol{\mu}_j$ is composed of n^j elements while $\mathbf{W}_j$ is a matrix of $n^j \times n^j$ so is $\mathbf{F}_j$. If we denote the element of $\mathbf{F}(\mathbf{x})$ at the intersection of its j_1th row and j_2th column by $F^{(j)}_{j_1,j_2}(\mathbf{x})$ we can write the following image Kronecker power series

$$F^{(j)}_{j_1,j_2}(\mathbf{x}) = \sum_{k=0}^{\infty} \mathbf{F}^{(j)\,T}_{j_1,j_2,k}\,[\,\boldsymbol{\Omega}(\mathbf{x})\,\mathbf{x}\,]^{\otimes k} = \sum_{k=0}^{\infty} [\,\boldsymbol{\Omega}(\mathbf{x})\,\mathbf{x}\,]^{\otimes k\,T}\,\mathbf{F}^{(j)}_{j_1,j_2,k} \tag{56}$$

which mean

$$\int_V dV \omega(\mathbf{x})\,F^{(j)}_{j_1,j_2}(\mathbf{x})\,[\boldsymbol{\Omega}(\mathbf{x})\,\mathbf{x}]^{\otimes j} = \int_V dV \omega(\mathbf{x})\,[\boldsymbol{\Omega}(\mathbf{x})\,\mathbf{x}]^{\otimes j}\,F^{(j)}_{j_1,j_2}(\mathbf{x})$$

$$= \sum_{k=0}^{\infty} \int_V dV \omega(\mathbf{x})\,[\boldsymbol{\Omega}(\mathbf{x})\,\mathbf{x}]^{\otimes j}\,[\boldsymbol{\Omega}(\mathbf{x})\,\mathbf{x}]^{\otimes k\,T}\,\mathbf{F}^{(j)}_{j_1,j_2,k} \tag{57}$$

If we define

$$\mathbf{M}_{j,k} \equiv \int_V dV \omega(\mathbf{x}) \left[\boldsymbol{\Omega}(\mathbf{x})\,\mathbf{x}\right]^{\otimes j} \left[\boldsymbol{\Omega}(\mathbf{x})\,\mathbf{x}\right]^{\otimes k^T}, \qquad j,k = 0,1,2,\ldots \tag{58}$$

then we can write

$$\sum_{k=0}^{\infty} \int_V dV \omega(\mathbf{x}) \left[\boldsymbol{\Omega}(\mathbf{x})\,\mathbf{x}\right]^{\otimes j} \left[\boldsymbol{\Omega}(\mathbf{x})\,\mathbf{x}\right]^{\otimes k^T} \mathbf{F}^{(j)}_{j_1,j_2,k} = \sum_{k=0}^{\infty} \mathbf{M}_{j,k} \mathbf{F}^{(j)}_{j_1,j_2,k} \tag{59}$$

which implies

$$\boldsymbol{\mu}_j = \sum_{j_1,j_2}^{n^j} \mathbf{e}_{j_1} \mathbf{e}^T_{j_2} \sum_{k=0}^{\infty} \mathbf{M}_{j,k} \mathbf{F}^{(j)}_{j_1,j_2,k}, \qquad j = 0,1,2,\ldots \tag{60}$$

Evidently, these equations involve denumerable infinitely many unknowns and only a few (n^j) of them can be expressed in terms of others. If the resulting expressions of those unknowns are used in the definition of the F definition then a linear combination of denumerable infinitely many matrix valued functions appears with arbitrary coefficients in the expressions. These should be linearly independent and may be used like a basis set for the generating function $\mathbf{W}_j$. We do not get into further details of this issue since we find this level of information sufficient for our purposes.

7 Concluding remarks

The primary focus of this study has been to extend the results of PEA for the determination of expectation value dynamics of quantum mechanical operators without explicitly solving Schrödinger equation. For this purpose, first a multivariate finite interval Hausdorff moment problem is defined to be able to get more appropriate forms for the analysis and algorithm developments of PEA. Necessary and sufficient conditions for the existence and the uniqueness of the solution to this problem is discussed. Solution methodology is given to that problem in rather broader mathematical details. This is the first contribution of this study.

Also, in this study, a matrix weighted Kronecker powers sequence has been taken into consideration as a multivariate finite interval Hausdorff-like moment problem to be able to model the correlations between expectation values of different kinds of quantum mechanical operators and thus to expect more accuracy and rapid convergence in the calculations. Necessary and sufficient conditions for the existence of the solution to this problem has also been discussed. Here we have used not the Kronecker powers of the system vector but its image under an appropriately given square matrix valued function of the system vector. This may bring more control for the approximations. This is the second important contribution of this study.

The third type moment problem like approach has been focused on the sequence whose elements involve order dependent matrix coefficients. This problem aims the evaluation of the order dependent moment like generating functions and certainly has denumerable infinitely many solutions. This infinitely many solution case generates infinitely many linearly independent matrix valued functions which can be used as basis function set.

The results presented here have two important aspects. The first one of these aspects is the usage of the weight functions generated from the moment problems suppress the divergent nature of the initial expectation values of the Kronecker powers of the system vector and thus PEA produces convergent series. The second aspect is that computational expense of the PEA can have a dramatic decrease because the sum of the series which are given in (18) and (19) does not require the explicit formation of the telescopic matrices whose dimensions increases by the powers of the terms taken from the series. Thus, this formulation requires less computational effort both in the sense of memory requirements and in the sense of necessary CPU time. Further details about implementation and computational requirements are left as a future work.

The results and the solutions obtained in this work can facilitate the analysis and the algorithm developments of the PEA for the quantum mechanical applications beside the systems whose initial conditions is not given with an accompanying Dirac delta initial probability density function.

The Stieltjes moment problem is expected to be one of our future work s in this presented framework. The another one of our future studies will be presumably the solution of the rectangular eigenvalue problem. Also, Padé summation of the divergent series produced by PEA can also be considered as future studies.

The companion of this paper focuses on the mathematical fluctuation theoretical aspects of the issues of this work.

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References

1. P. Hohenberg, W. Kohn, Inhomogeneous electron gas. Phys. Rev. **136**, B864–B871 (1964)
2. W. Kohn, L.J. Sham, Self-consistent equations including exchange and correlation effects. Phys. Rev. **140**, A1133–A1138 (1965)
3. C. Huang, E.A. Carter, Nonlocal orbital-free kinetic energy density functional for semiconductors. Phys. Rev. B **81**, 045206-1–045206-15 (2010)
4. L. Hung, E.A. Carter, Accurate simulations of metals at the mesoscale: explicit treatment of 1 million atoms with quantum mechanics. Chem. Phys. Lett. **475**, 163–170 (2009)
5. L. Hung, E.A. Carter, Orbital-free DFT simulations of elastic response and tensile yielding of ultrathin [111] Al nanowires. J. Phys. Chem. C **115**, 6269–6276 (2011)
6. M.G. Reuter, L.-W. Wang, Quantum mechanics without wavefunctions. SIAM News **46**(5) (2013). http://www.siam.org/pdf/news/2073.pdf
7. M. Ayvaz, M. Demiralp, Probabilistic evolution approach to the expectation value dynamics of quantum mechanical operators, part II: the use of mathematical fluctuation theory. J. Math. Chem. (under review)
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 co nicality, 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 trilogy, part 2: spectral issues for block triangular evolution mat rix, 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). (2013). doi:10.1007/s10910-013-0298-5
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. B. Fuglede, The multidimensional moment problem. Exp. Math. **1**, 47–65 (1983)
18. N.I. Akhiezer, *The Classical moment Problem and Some Related Questions in Analysis. University Mathematical Monographs* (Hafner Publishing Company, New York, 1965)
19. F. Hausdorff, Summationsmethoden und Momentfolgen. I. Mathematische Zeitschrift **9**, 74–109 (1921)
20. F. Hausdorff, Summationsmethoden und Momentfolgen. II. Mathematische Zeitschrift **9**, 280–299 (1921)