

A probabilistic evolution approach trilogy, part 3: temporal variation of state variable expectation values from Liouville equation perspective

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Abstract This is the third and therefore the final part of a trilogy on probabilistic evolution approach. The work presented here focuses on the probabilistic evolution determination for the state variables of a many particle system from classical mechanical point of view. Probabilistic evolution involves the expected value evolutions for all natural number Kronecker powers of the state variables, positions and momenta. We use the phase space distribution of the Liouville equation perspective to construct the expected values of the state variables' Kronecker powers to define unknown temporal functions. The infinite number homogeneous linear ODEs with an infinite constant coefficient matrix are constructed by following the same steps as in the previous two works on quantum mechanics. The only difference is in the definitions of the expected values here. We also focus on a system of many harmonic oscillators to illustrate the block triangularity.

Keywords Probabilistic evolution · Expected value dynamics · Evolution matrix · Phase space distribution · Elastic spring forces

1 Introduction

The classical dynamical equations of motion can be constructed by using various formalisms like Hamilton's where the equations are derived from a function of state variables, called "Hamiltonian", which somehow corresponds to the total energy of the system under consideration. If we consider a classical system composed of some

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number of particles such that the degree of freedom is at most three times the number of the particles and this degree may decrease if certain number of bounds exist amongst the particles. If we denote the degree of freedom by N then each freedom is characterized by a position and a momentum variable (conjugate variables). If we denote the position and momentum for the j th degree of freedom by q_j and p_j ($j = 1, 2, \dots, N$) respectively then the system Hamiltonian depends on these N variables, that is,

$$H = H(p_1, \dots, p_N, q_1, \dots, q_N) \tag{1}$$

where we have assumed autonomy (that is, time independence) in the Hamiltonian. The equations of motion can be written as follows in Hamilton formalism

$$\dot{p}_j = -\frac{\partial H}{\partial q_j}, \quad \dot{q}_j = \frac{\partial H}{\partial p_j}, \quad j = 1, 2, \dots, N \tag{2}$$

which define a trajectory in the $2N$ dimensional phase space spanned by positions and momenta when the beginning point of the trajectory is specified.

The autonomy donates the constancy to the Hamiltonian when the system moves along a trajectory. In other words, the value of the Hamiltonian is conserved during the system’s evolution. This happens only when the system under consideration does not interact with the external agents. Otherwise the Hamiltonian becomes explicitly dependent on time. Then the energy exchange occurs between the system and its environment. Thus, only isolated systems can conserve their total energies. We will focus only on the energy conserving systems here for simplicity.

Trajectory evaluations become unfeasible when the number of particles climbs up to huge values like Avogadro’s number. Even rather smaller values like hundreds or thousands may create technical problems. Hence, statistical methods can be considered for large values of N . To this end $2N$ dimensional phase space, which is spanned by p s and q s, can be used to focus on not individual particles but their distribution in this space. We define a phase space distribution function denoted by $\rho(\mathbf{p}, \mathbf{q}, t)$ such that its product with the hypervolume element of this $2N$ dimensional space, $dV = dp_1 \dots dp_N dq_1 \dots dq_N$ corresponds to the probability that the system’s positions and momenta lie in the hypervolume element $dV = dp_1 \dots dp_N dq_1 \dots dq_N$. Since the total derivative of ρ in time should vanish (population should be constant as long as no creation and annihilation occurs), the following equation must be satisfied

$$i \frac{\partial \rho(\mathbf{p}, \mathbf{q}, t)}{\partial t} = \widehat{L} \rho(\mathbf{p}, \mathbf{q}, t) \tag{3}$$

which is called Liouville equation for historical reasons. It is a first order partial differential equation and uniquely defines the time evolution of the many particle system under consideration when the initial probability distribution of the system is specified. The operator \widehat{L} appearing in this equation, is explicitly defined as follows

$$\widehat{L} \equiv -i \sum_{j=1}^N \left[\frac{\partial H}{\partial p_j} \frac{\partial}{\partial q_j} - \frac{\partial H}{\partial q_j} \frac{\partial}{\partial p_j} \right] \tag{4}$$

This particular structure gives a Hermitian nature to this operator as long as the Hamiltonian remains continuous throughout the integration domain which is generally an entire phase space unless certain limitations are imposed on the domains of the state variables.

The Hamiltonian of the system depends on $2N$ number of state variables, N number of positions and N number of momenta so does the distribution function. Any function of state variables can be averaged by using the above mentioned distribution function over the entire phase space (or its certain subregion if there exist some restrictions). These averaged values or in other words expected values depend on the expected values of not only the state variables but also all their natural number Kronecker powers as long as the Hamiltonian can be expanded to a Taylor series. Hence it is quite meaningful to attempt to construct ODEs for the expected values of the Kronecker powers of the state variables. We do this here by following a route which is very similar to the ones in the case of explicit ODEs and quantum mechanics of previous two parts of this trilogy. For illustrative reasons we also try to solve the obtained set of ODEs under given initial conditions for a system of particles interacting through elastic forces (harmonic oscillators).

Paper is organised as follows. The second section covers the construction of the so-called “Probabilistic Evolution Equations” while the third section recalls the construction of truncation approximants and their convergence as it is done for the quantum mechanical systems. The fourth section involves the solution of the probabilistic evolution equations for a system of harmonic oscillators. The fifth section focuses on the initial conditions together with certain properties of the system’s evolution. The sixth section gives implementation just for illustration while the seventh section finalizes the paper with concluding remarks.

2 Probabilistic evolution equations (PEEs)

In this section we take into consideration the system in its quite general form. If we denote the degree of freedom of the system by n_d then we can define the following state vector

$$\mathbf{s} \equiv [p_1 \dots p_{n_d} q_1 \dots q_{n_d}]^T \quad (5)$$

whose Kronecker square (Kronecker product with itself) is explicitly defined as

$$\mathbf{s}^{\otimes 2} \equiv \mathbf{s} \otimes \mathbf{s} \equiv [p_1 \mathbf{s}^T \dots p_{n_d} \mathbf{s}^T \quad q_1 \mathbf{s}^T \dots q_{n_d} \mathbf{s}^T]^T \quad (6)$$

which can be generalized to

$$\begin{aligned} \mathbf{s}^{\otimes m} &\equiv \mathbf{s} \otimes \mathbf{s}^{\otimes(m-1)} \\ &\equiv [p_1 \mathbf{s}^{\otimes(m-1)T} \dots p_{n_d} \mathbf{s}^{\otimes(m-1)T} \quad q_1 \mathbf{s}^{\otimes(m-1)T} \dots q_{n_d} \mathbf{s}^{\otimes(m-1)T}] \\ m &= 1, 2, 3, \dots \end{aligned} \quad (7)$$

where the zeroth Kronecker power produces the universal scalar, just 1 (truly speaking it is a single element vector), by definition.

Now the expected value of the m th Kronecker power of the state vector can be given as follows

$$\langle \mathbf{s}^{\otimes m} \rangle (t) \equiv \int_V dV \rho(\mathbf{p}, \mathbf{q}, t) \mathbf{s}^{\otimes m}, \quad m = 1, 2, 3, \dots \tag{8}$$

where the integration domain V is generally whole phase space and the state variables under integration does not temporally vary since they just play the role of dummy variable of integration. The time differentiation of both sides in this equation gives

$$\begin{aligned} \frac{d \langle \mathbf{s}^{\otimes m} \rangle (t)}{dt} &= \int_V dV \frac{\partial \rho(\mathbf{p}, \mathbf{q}, t)}{\partial t} \mathbf{s}^{\otimes m}, = \int_V dV \{ -i \widehat{L} \rho(\mathbf{p}, \mathbf{q}, t) \} \mathbf{s}^{\otimes m} \\ &= \int_V dV \rho(\mathbf{p}, \mathbf{q}, t) \{ -i \widehat{L} (\mathbf{s}^{\otimes m}) \}, \quad m = 1, 2, 3, \dots \end{aligned} \tag{9}$$

where we have used the Liouville equation given in (3) and the Hermiticity of \widehat{L} . The first order homogeneous partial differential operator of \widehat{L} enables us to use Leibnitz rule for the evaluation of its action on a product composed of a finite number of factors and therefore to obtain

$$\widehat{L} (\mathbf{s}^{\otimes m}) = \sum_{k=0}^{m-1} \mathbf{s}^{\otimes k} \otimes (\widehat{L} \mathbf{s}) \otimes \mathbf{s}^{\otimes (m-k-1)} \tag{10}$$

which urges us to focus on the vector $(\widehat{L} \mathbf{s})$. We can write

$$-i \widehat{L} \mathbf{s} = \begin{bmatrix} \nabla_{\mathbf{q}} H \\ -\nabla_{\mathbf{p}} H \end{bmatrix} \tag{11}$$

where $\nabla_{\mathbf{p}}$ and $\nabla_{\mathbf{q}}$ denote the gradients of the Hamiltonian with respect to the momentum and position variables. The use of this result in (10) and therefore in (9) enables us to get a much more explicit expression at the right hand side. We obtain

$$\frac{d \langle \mathbf{s}^{\otimes m} \rangle (t)}{dt} = \left\langle \sum_{k=0}^{m-1} \mathbf{s}^{\otimes k} \otimes \begin{bmatrix} \nabla_{\mathbf{q}} H \\ -\nabla_{\mathbf{p}} H \end{bmatrix} \otimes \mathbf{s}^{\otimes (m-k-1)} \right\rangle (t) \tag{12}$$

which can be put into more amenable form by expanding the momentum and position gradients of the Hamiltonian to Kronecker powers of the system vector. By doing so, the right hand side of this equation can be expressed as an infinite linear combination of the expected values of the system vector Kronecker powers. By gathering all equations obtained in this manner for all natural number values of m an infinite set of ODEs is obtained. This set is first order and linear with a constant infinite matrix coefficient. To explicitly show what really happens we can define the following expansion first

$$-i\widehat{L}s = \begin{bmatrix} \nabla_q H \\ -\nabla_p H \end{bmatrix} \equiv \sum_{j=0}^{\infty} \mathbf{L}_j s^{\otimes j} \tag{13}$$

where the constant coefficient \mathbf{L}_j is a matrix of $n_d \times n_d^j$. It is completely determined by the system Hamiltonian. This definition enables us to rewrite (12) as follows

$$\begin{aligned} \frac{d \langle s^{\otimes m} \rangle (t)}{dt} &= \left\langle \sum_{k=0}^{m-1} s^{\otimes k} \otimes \left[\sum_{j=0}^{\infty} \mathbf{L}_j s^{\otimes j} \right] \otimes s^{\otimes (m-k-1)} \right\rangle (t) \\ &= \sum_{j=0}^{\infty} \sum_{k=0}^{m-1} \left\langle s^{\otimes k} \otimes \left[\mathbf{L}_j s^{\otimes j} \right] \otimes s^{\otimes (m-k-1)} \right\rangle (t) \\ &= \sum_{j=0}^{\infty} \sum_{k=0}^{m-1} \left(\mathbf{I}_{n_d}^{\otimes k} \otimes \mathbf{L}_j \otimes \mathbf{I}_{n_d}^{\otimes (m-k-1)} \right) \langle s^{\otimes (m+j-1)} \rangle (t) \\ &= \sum_{j=m-1}^{\infty} \sum_{k=0}^{m-1} \left(\mathbf{I}_{n_d}^{\otimes k} \otimes \mathbf{L}_{j-m+1} \otimes \mathbf{I}_{n_d}^{\otimes (m-k-1)} \right) \langle s^{\otimes j} \rangle (t) \end{aligned} \tag{14}$$

which urges us to define the following block matrices

$$\mathbf{E}_{m,j} \equiv \sum_{k=0}^{m-1} \mathbf{I}_{n_d}^{\otimes k} \otimes \mathbf{L}_{j-m+1} \otimes \mathbf{I}_{n_d}^{\otimes (m-k-1)}, \quad m, j = 0, 1, 2, \dots \tag{15}$$

where \mathbf{I}_{n_d} stands for the $n_d \times n_d$ type identity matrix. These block matrices vanish if j is less than $m - 1$.

We can now rewrite (14) as follows

$$\frac{d \langle s^{\otimes m} \rangle (t)}{dt} = \sum_{j=0}^{\infty} \mathbf{E}_{m,j} \langle s^{\otimes j} \rangle (t), \quad m = 0, 1, 2, \dots \tag{16}$$

which urges us to define

$$\xi(t) \equiv \begin{bmatrix} \langle s \rangle^{\otimes 0}(t) \\ \vdots \\ \langle s \rangle^{\otimes j}(t) \end{bmatrix}, \quad \mathbf{E} \equiv \begin{bmatrix} \mathbf{E}_{0,0} & \cdots & \mathbf{E}_{0,j} & \cdots \\ \vdots & \ddots & \vdots & \cdots \\ \mathbf{E}_{j,0} & \cdots & \mathbf{E}_{j,j} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \tag{17}$$

and to get the following concise infinite vector equation instead of (16)

$$\dot{\xi}(t) = \mathbf{E}\xi(t). \tag{18}$$

This is an infinite linear and homogeneous vector ODE whose infinite coefficient matrix is constant. We call \mathbf{E} “Evolution Matrix” by following the same reasonings in our previous works for explicit ODEs and quantum mechanics. As can be easily noticed from above discussions, this matrix is in upper block Hessenberg form. Its each block diagonal is generated from a separate coefficient of the Kronecker power series of $i\widehat{L}s$. In this sense, the coefficients \mathbf{L}_0 and \mathbf{L}_1 play important roles. \mathbf{L}_0 generates the blocks of the lower adjacent neighbor of the main diagonal. If it vanishes then the Evolution Matrix becomes upper block triangular. This facilitates many analyses about the Evolution Matrix, especially its spectral entities. \mathbf{L}_0 is a vector of n_d elements and it vanishes on the minima of the potential function as we mentioned above.

\mathbf{L}_1 is a square matrix of n_d^2 elements and generates all elements of the main diagonal of Evolution Matrix. Hence, its spectrum determines the spectrum of the Evolution Matrix when it is upper block triangular. We have investigated this issue in more detail in the second part of this trilogy and therefore we do not repeat the same or very similar things here. The only difference between the previous and present cases is the structural differences in the coefficient matrices \mathbf{H} s and \mathbf{L} s.

Even though the triangularity facilitates many things very much the construction of the truncation approximants and investigation of their convergence still remain rather complicated. This comes from the nonsparse structure of the Evolution Matrix. Sparsity becomes very fruitful if it corresponds to diagonality which can be obtained in very simple systems like the system of harmonic oscillators only. These systems are generally very well known although there may still be some gates open for investigation. Beyond diagonality the simplest sparse case appears when the Evolution Matrix has only main block diagonal and adjacent block diagonal neighbor. We call these cases “Conical” since they come from the descriptive functions which are multinomials with at most second degree. We have investigated the truncation approximants and their convergence for this case in the first part of this trilogy. Hence we are not willing to retrace the same route here.

3 Probabilistic evolution equations for a classical harmonic oscillator system

To get concreteness we need to specify the system and therefore the Hamiltonian. In this work we focus on a system of quantum harmonic oscillators. We can explicitly write the Hamiltonian for the system composed of N particles interacting through elastic forces as follows

$$H \equiv \sum_{j=1}^N \frac{1}{2m_j} \left(p_{3j-2}^2 + p_{3j-1}^2 + p_{3j}^2 \right) + V(q_1, \dots, q_{3N}) \quad (19)$$

where N stands for the number of the particles while parameters m_j denote the masses of the particles. The potential function V is specified as follows

$$\begin{aligned}
 V(q_1, \dots, q_{3N}) &\equiv \frac{1}{2} \sum_{\substack{j,k=1 \\ k>j}}^N \kappa_{j,k} \left[(q_{3j-2} - q_{3k-2})^2 + (q_{3j-1} - q_{3k-1})^2 \right. \\
 &\quad \left. + (q_{3j} - q_{3k})^2 \right] \\
 &= \frac{1}{2} \mathbf{q}^T (\mathbf{K} \otimes \mathbf{I}_3) \mathbf{q}
 \end{aligned} \tag{20}$$

where $\kappa_{j,k}$ s are the elastic force constants while \mathbf{I}_3 and \mathbf{q} denote the 3×3 identity matrix and the $3N$ element position vector composed of q s, respectively. The matrix \mathbf{K} (we may call this symmetric matrix “Elasticity Matrix”) has the following general diagonal and off-diagonal elements

$$K_{j,j} \equiv \sum_{k=1}^{j-1} \kappa_{k,j} + \sum_{k=j+1}^N \kappa_{j,k}, \quad j = 1, 2, \dots, N \tag{21}$$

$$K_{j,k} \equiv -\kappa_{j,k}, \quad 1 \leq j < k \leq N \tag{22}$$

(20) reveals the quadratic form structure of the potential in the position variables. The kinetic energy part of the Hamiltonian is also a quadratic form but not in positions, instead in momenta. To show this we can define the mass matrix \mathbf{M} whose general term $M_{j,k}$ is given as

$$M_{j,k} \equiv m_j \delta_{j,k}, \quad 1 \leq j, k \leq N \tag{23}$$

where $\delta_{j,k}$ stands for the Kronecker’s delta symbol. All these enable us to write

$$\begin{aligned}
 H &\equiv \sum_{j=1}^N \frac{1}{2} \mathbf{p}^T (\mathbf{M}^{-1} \otimes \mathbf{I}_3) \mathbf{p} + \frac{1}{2} \mathbf{q}^T (\mathbf{K} \otimes \mathbf{I}_3) \mathbf{q} \\
 &\equiv \mathbf{s}^T \mathbf{H}_K \mathbf{s}
 \end{aligned} \tag{24}$$

where

$$\begin{aligned}
 \mathbf{p} &\equiv [p_1 \dots p_{3N}]^T \\
 \mathbf{q} &\equiv [q_1 \dots q_{3N}]^T \\
 \mathbf{s} &\equiv [p_1 \dots p_{3N} \ q_1 \dots q_{3N}]^T \\
 \mathbf{H}_K &\equiv \begin{bmatrix} \frac{1}{2} (\mathbf{M}^{-1} \otimes \mathbf{I}_3) & \mathbf{0} \\ \mathbf{0} & \frac{1}{2} (\mathbf{K} \otimes \mathbf{I}_3) \end{bmatrix}.
 \end{aligned} \tag{25}$$

We call \mathbf{H}_K “The Hamiltonian Kernel Matrix”. It takes the responsibility of identifying the system under consideration via mass and force constant parameters.

Now we can write

$$\nabla_{\mathbf{p}} H = (\mathbf{M}^{-1} \otimes \mathbf{I}_3) \mathbf{p} \tag{26}$$

$$\nabla_{\mathbf{q}} H = (\mathbf{K} \otimes \mathbf{I}_3) \mathbf{q} \tag{27}$$

This urges us to define

$$\mathbf{S} \equiv \begin{bmatrix} \mathbf{0} & \mathbf{K} \otimes \mathbf{I}_3 \\ -\mathbf{M}^{-1} \otimes \mathbf{I}_3 & \mathbf{0} \end{bmatrix} \tag{28}$$

which is a very important entity we call ‘‘System Matrix’’. (26), (27), and, (28) lead us to write

$$\begin{bmatrix} \nabla_{\mathbf{q}} H \\ -\nabla_{\mathbf{p}} H \end{bmatrix} = \mathbf{S} \mathbf{s} \tag{29}$$

This converts (12) to the following equation

$$\frac{d \langle \mathbf{s}^{\otimes m} \rangle (t)}{dt} = \left\langle \sum_{k=0}^{m-1} \mathbf{s}^{\otimes k} \otimes (\mathbf{S} \mathbf{s}) \otimes \mathbf{s}^{\otimes (m-k-1)} \right\rangle \tag{30}$$

where the use of the distributive property of matrix product over the Kronecker product enables us to write

$$\frac{d \langle \mathbf{s}^{\otimes m} \rangle (t)}{dt} = \mathbf{S}_m \langle \mathbf{s}^{\otimes m} \rangle (t) \tag{31}$$

where

$$\begin{aligned} \mathbf{S}_m &\equiv \sum_{k=0}^{m-1} \mathbf{I}_{6N}^{\otimes k} \otimes \mathbf{S} \otimes \mathbf{I}_{6N}^{\otimes (m-k-1)} = \sum_{k=0}^{m-1} \mathbf{S}_{m,k} \\ \mathbf{S}_{m,k} &\equiv \mathbf{I}_{6N}^{\otimes k} \otimes \mathbf{S} \otimes \mathbf{I}_{6N}^{\otimes (m-k-1)}, \quad k = 0, 1, 2, \dots, m - 1 \end{aligned} \tag{32}$$

In these formulae \mathbf{I}_{6N} stands for the $6N \times 6N$ identity matrix. A Kronecker power of an identity matrix is also an identity matrix whose number of rows (or columns) is equal to the product of the original identity matrix number of rows (or columns) multiplied by the Kronecker power. Thus,

$$\mathbf{S}_{m,k} = \mathbf{I}_{6Nk} \otimes \mathbf{S} \otimes \mathbf{I}_{6N(m-k-1)}, \quad k = 0, 1, 2, \dots, m - 1 \tag{33}$$

can be used for a concise result when it is necessary. However we will prefer to widely use (32) because of its convenience in evaluations.

The formal explicit solution of (31) can be written as follows

$$\langle \mathbf{s}^{\otimes m} \rangle (t) = e^{t \mathbf{S}_m} \langle \mathbf{s}^{\otimes m} \rangle (0) \tag{34}$$

which uniquely determines the expected value of the m th Kronecker power of the system vector in time when this expected value's initial value is specified. Since a careful and simple analysis shows that $\mathbf{S}_{m,k}$ matrices are mutually commutative, one can write

$$e^{t\mathbf{S}_m} = \prod_{k=0}^{m-1} e^{t\mathbf{S}_{m,k}} \quad (35)$$

and, as can be verified through powering and series expansion,

$$e^{t\mathbf{S}_{m,k}} = \mathbf{I}_{6N}^{\otimes k} \otimes e^{t\mathbf{S}} \otimes \mathbf{I}_{6N}^{\otimes(m-k-1)}, \quad (36)$$

it finally gives

$$e^{t\mathbf{S}_m} = \left[e^{t\mathbf{S}} \right]^{\otimes m} \quad (37)$$

and therefore

$$\langle \mathbf{s}^{\otimes m} \rangle (t) = \left[e^{t\mathbf{S}} \right]^{\otimes m} \langle \mathbf{s}^{\otimes m} \rangle (0) \quad (38)$$

As can be immediately noticed the system matrix \mathbf{S} is the most fundamental component of the probabilistic evolution. Hence its spectrum has also great significance on the behaviour of the system under consideration. A rather simple but comprehensive analysis shows that the entire spectrum of this matrix resides on the imaginary axis of the complex eigenvalue plane under a symmetry with respect to the origin. This feature gives trigonometrically oscillating nature to the probabilistic evolutions for all m values. Thus, the image of the initial value vector under the exponential of this matrix multiplied by time, creates just oscillations without decaying or exploding when time tends to go to infinity.

4 Focusing on the initial values

Let us define

$$\langle \mathbf{s} \rangle (0) \equiv \mathbf{s}_{in} = [a_1 \dots a_{3N} \ b_1 \dots b_{3N}]. \quad (39)$$

If the initial distribution were strictly sharply localized, that is, a product of certain delta distributions then we would say that “There is no initial fluctuation”. In this case we could write the fluctuation free expected value of the m th Kronecker power of the system vector as follows

$$\langle \mathbf{s}^{\otimes m} \rangle_{nofluc} (t) = \left[e^{t\mathbf{S}} \right]^{\otimes m} \mathbf{s}_{in}^{\otimes m} = \left[e^{t\mathbf{S}} \mathbf{s}_{in} \right]^{\otimes m} \quad (40)$$

which would be composed of just a single evolution through Kronecker powers. Whereas, the real situation involves the initial distributions which are not characterized by delta functions. Hence, the following formula becomes valid

$$\langle \mathbf{s}^{\otimes m} \rangle (t) = \langle \mathbf{s}^{\otimes m} \rangle_{nofluc} (t) + \left[e^{t\mathbf{S}} \right]^{\otimes m} \left[\langle \mathbf{s}^{\otimes m} \rangle (0) - \mathbf{s}_{in}^{\otimes m} \right] \tag{41}$$

where the rightmost entity between the left and the right brackets describes the fluctuation in the initial values. This fluctuation depends on the initial distribution. In this work we will focus only on Gaussian wave packets where the initial distribution’s function form is given as follows

$$\rho (\mathbf{p}, \mathbf{q}, 0) \equiv \left[\prod_{j=1}^{3N} \frac{1}{\sqrt{2\pi\sigma_{p,j}}} e^{-\frac{(p_j-a_j)^2}{2\sigma_{p,j}}} \right] \times \left[\prod_{j=1}^{3N} \frac{1}{\sqrt{2\pi\sigma_{q,j}}} e^{-\frac{(q_j-b_j)^2}{2\sigma_{q,j}}} \right] \tag{42}$$

which apparently produces (39) and, beyond that, the following simple fluctuation equalities

$$\langle p_j^2 \rangle - \langle p_j \rangle^2 = \sigma_{p,j}, \quad \langle q_j^2 \rangle - \langle q_j \rangle^2 = \sigma_{q,j}, \quad j = 1, 2, \dots, 3N \tag{43}$$

Even though much higher order fluctuations can be evaluated accordingly in terms of the parameters $as, bs,$ and σs we will not attempt to deal with them here since it is out of the scope of this work.

The distribution function’s initial form is normalized to produce 1 when it is integrated over the whole phase space. Hence it corresponds to the percentage of being in an infinitesimal hypervolume element located at the point characterized by its arguments in the phase space. We can use a coordinate transformation over momentum and position variables as follows to facilitate the analysis

$$p_j = a_j + \sqrt{2\sigma_{p,j}}u_{p,j}, \quad q_j = b_j + \sqrt{2\sigma_{q,j}}u_{q,j}, \quad j = 1, 2, \dots, 3N \tag{44}$$

These affine transformations change the state vector as follows

$$\mathbf{s} = \mathbf{s}_{in} + \sqrt{2}\mathbf{\Sigma}\mathbf{u} \tag{45}$$

where $\mathbf{\Sigma}$ is a diagonal matrix composed of the square roots of the σ parameters in the order of state variables while \mathbf{u} stands for a vector whose elements are us ordered accordingly.

The employment of (45) in the deviation term at the right hand side in (41) permits us to write

$$\langle \mathbf{s}^{\otimes m} \rangle (0) - \mathbf{s}_{in}^{\otimes m} = \sqrt{2} \sum_{j=0}^{m-1} \mathbf{s}_{in}^{\otimes j} \otimes (\mathbf{\Sigma} \langle \mathbf{u} \rangle) \otimes \mathbf{s}_{in}^{\otimes (m-j-1)} + \dots \tag{46}$$

where the remainder terms of the right hand side have more than one appearances of the matrix Σ . As can be noticed easily the expected value of the vector \mathbf{u} vanishes. This urges us to rewrite (46) as

$$\langle \mathbf{s}^{\otimes m} \rangle (0) - \mathbf{s}_{in}^{\otimes m} = \sum_{j=0}^{\ell-1} \sum_{k=0}^{m-1} \mathbf{s}_{in}^{\otimes j} \otimes \left\langle (\Sigma \mathbf{u}) \otimes \mathbf{s}_{in}^{\otimes k} \otimes (\Sigma \mathbf{u}) \right\rangle \otimes \mathbf{s}_{in}^{\otimes (m-j-k-2)} + \dots \quad (47)$$

where leading terms do not vanish now and they are proportional to the fluctuations. The remainder terms having odd number of appearances of Σ at the right hand side in (47) vanish because of the vanishing expected values of odd Kronecker powers of \mathbf{u} . Hence, the series expansion at the right hand side of this equality never contains square roots of the fluctuations. We do not intend to explicitly focus on the remainder terms here since this issue is rather a technicality.

The expected value of the m th Kronecker power of \mathbf{u} contains terms proportional to $m!$ when m is even. This means that the $2m$ th terms of (47) at the right hand side very rapidly grows when m tends to go to infinity. This makes the expansion in ascending number of appearances of Σ divergent although a certain level of asymptoticity can be used. So, even small fluctuations in state variable expected values may cause rapid growth and therefore deviation from the fluctuation free case in the expected values of the Kronecker powers of the state vector. We find this level of information sufficient for our purposes here.

5 Numerical implementation

In this chapter, we organize an example to show the details of our new method numerically. For this purpose, a computer program is written in MuPAD and is executed within 10-digit precision to obtain the numerical results.

In the example, for simplicity, we use 2 particles and we compose the expected value of the 0th Kronecker power of the state vector with the help of the Gauss wave packets by using relation (42).

Relation (7) allows us to evaluate the m th Kronecker power of the state vector while the expected value of the m th outer power of the state vector is evaluated through relation (8).

Next step is to build the system matrix and elasticity matrix for defining the dynamics of the system. Relations (21) and (28) are given for this purpose. Finally, the relation (38) makes it possible to obtain the probabilistic evolution of the system by using the system matrix and relations (35) and (37).

Figure 1 shows how the expected value of the initial state vector changes over time with the help of function norm. Here, the red and blue curves represent the norm of the function of the initial state vector's expected value and the norm of the function of the 2nd outer power of the state vector. Since we use norm procedure, it defines overall change over time. The purpose here has been to show the mathematical fluctuation effects on the evolution in a quite concise manner. Of course, much more comprehensive scriptings can be used to this end even though we do not intend to do so here.

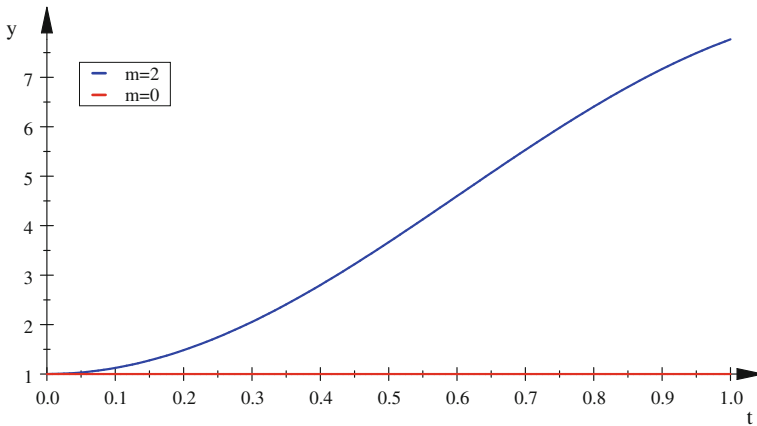


Fig. 1 Norm variations of the initial state vector and the second outer (Kronecker) power of the state vector

6 Conclusion

In this work we have focused on the expected values of the state vector Kronecker powers to determine the probabilistic evolution of a system governed by the Liouville equation. Even though the formulation is given at a quite general level by addressing to the first and second parts of this trilogy we have taken a system of particles interacting via elastic forces. In other words, we have focused on a system of Harmonic Oscillators. We have constructed the expected value evolutions for each Kronecker power of the state vector separately. Then we have discussed on the fluctuations in the initial values. We enumerate the concluding remarks below

1. The evolution ODE for the m th Kronecker power of the state vector involves only this power due to the very particular structure of the harmonic oscillators. This might not be the case for other types of systems. In more complicated systems the ODE involving the temporal derivative of the m th Kronecker power of the state vector may be equal to a sum over some or all possible Kronecker power expected values of the state vector. This gathers the ODEs for all m values into a single infinite vector ODE which is linear in the state vector expected values with a constant infinite coefficient matrix.
2. The infinite vector ODE's coefficient we call "Evolution Matrix" has an upper blockwise Hessenberg form which can become blockwise triangular when certain vanishing conditions are satisfied in certain Hamiltonian related entities. Triangularity facilitates the analysis pretty much.
3. Even though we have not mentioned here the distribution function, for the system of harmonic oscillators considered here it can be found if the initial distribution is in Gaussian form. It is also in a Gaussian form. Depending on the fluctuations the distribution may loose its sharpness. That is, the probability density may spread out.
4. The asymptotic nature of the expansion in Σ signals out the invalidity of this expansion and urges us to use some other type of expansion or we can use

fluctuationlessness theorem to this end. Certain details of this issue have been given in the first part of this trilogy.

5. The Gaussian form given here is rather restricted since it involves only the fluctuations amongst the power expected values of each individual state variable separately. We could use a more general quadratic form structure where the inverse of the kernel matrix somehow corresponds to the fluctuations amongst all possible interactions between the state variables.
6. The analysis here can be extended to some other cases where the initial conditions may have much greater number of parameters which facilitate the controlling of the fluctuations.

These and some other issues will be the core topics of our future works.

Some references which are related to the authors' group works [1–9] and certain ODE related resources [10–14], together with a computer algebra system tutorial [15], are given in the references without any addressing in the text body since these papers' organisation is self-consistent and self-containing.

References

1. 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)
2. E. Demiralp, M. 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)
3. 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](https://doi.org/10.1007/s10910-012-0070-2)
4. M. Demiralp, E. Demiralp, A contemporary linear representation theory for ordinary differential equations: multilinear algebra in folded arrays (folars) perspective and its use in multidimensional case. *J. Math. Chem.* (2012). doi:[10.1007/s10910-012-0064-0](https://doi.org/10.1007/s10910-012-0064-0)
5. M. Demiralp, Fluctuationlessness theorem to approximate univariate functions' matrix representations. *SEAS Trans. Math.* **8**, 258–267 (2009)
6. C. Gözükrımı, M. Demiralp, The application of the fluctuation expansion with extended basis set to numerical integration. *WSEAS Trans. Math.* **8**, 205–212 (2009)
7. M. Demiralp, No fluctuation approximation in any desired precision for univariate matrix representations. *J. Math. Chem.* **47**, 99–110 (2010)
8. N. Altay, M. Demiralp, Numerical solution of ordinary differential equations by Fluctuationlessness Theorem. *J. Math. Chem.* **47**, 1323–1344 (2010)
9. M. Demiralp, Data production for a multivariate function on an orthogonal hyperprismatic grid via fluctuation free matrix representation: completely filled grid case. *IJEECE* **1**, 61–76 (2010)
10. E. Hairer, S.P. Nørsett, G. Wanner, *Solving Ordinary Differential Equations I: Nonstiff Problems*, (Springer, Berlin, 1993) (ISBN 978-3-540-56670-0)
11. E. Hairer, G. Wanner, *Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems*, 2nd edn. (Springer, Berlin, 1996) (ISBN 978-3-540-60452-5)
12. J. Vigo-Aguiar, M.J. Ferrández, VSVO multistep formulae adapted to perturbed second-order differential equations. *Appl. Math. Lett.* **11**(3), 83–87 (1998)
13. J.C. Butcher, *Numerical Methods for Ordinary Differential Equations* (Wiley, New York, 2003) (ISBN 978-0-471-96758-3)
14. J. Stoer, R. Bulirsch, *Introduction to Numerical Analysis*, 3rd edn. (Springer, Berlin, 2002) (ISBN 978-0-521-88068-8)
15. W. Oevel, F. Postel, S. Wehmeier, J. Gerhard, *The MuPAD Tutorial* (Springer, New York, 2000)