

A probabilistic evolution approach trilogy, part 2: spectral issues for block triangular evolution matrix, singularities, space extension

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Received: 9 August 2012 / Accepted: 2 September 2012 / Published online: 19 October 2012
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Abstract This is the second part of the trilogy on the probabilistic evolution approach and related to the quantum dynamical systems as the first part is. In this sense this work extends the content of the first part to the perhaps secondary but very important details. The spectral investigation of the evolution matrix reveals important issues first and brings the importance of the zero eigenvalues to the surface. The asymptotic convergence possibility and difficulties arising from there can be softened by redefining the state vector. Beside the redefinition, the dimensional extension by adding new elements to the state vector may facilitate the utilization of evolution matrix by bringing conicality or at least multinomiality. The space extension may also help us to deal with singular Hamiltonian systems. All these issues are focused on rather phenomenologically. Illustrative or not, no comprehensive implementation is given since the main purpose is just conceptuality.

Keywords Probabilistic evolution equations · Quantum expected values · Coordinate transforms · Space extension · Singular Hamiltonians

1 Introduction

Probabilistic evolution equations [1–4] and their solution is a quite new approach to solve explicit ODEs, and also PDEs via expectation values [5] as long as they can be defined. This approach extends the space to an infinite one by using the integer

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Kronecker powers of the state vector. Then an infinite set of ordinary differential equations (ODEs) is constructed such that it is linear and has an infinite constant coefficient matrix. This facilitates the theory however at the expense of dealing with infinitely many items.

We start with the definition of the expected value of a given operator \widehat{O} as follows

$$\begin{aligned} \frac{d\langle\widehat{O}\rangle(t)}{dt} &= \int_V dV \psi(\mathbf{x}, t)^* \left\{ \frac{i}{\hbar} [\widehat{H}\widehat{O} - \widehat{O}\widehat{H}] \right\} \psi(\mathbf{x}, t) \\ &= \left\langle \frac{i}{\hbar} [\widehat{H}\widehat{O} - \widehat{O}\widehat{H}] \right\rangle \end{aligned} \quad (1)$$

where \widehat{H} and $\psi(\mathbf{x}, t)$ stand for the system Hamiltonian and the wave function while V and dV denote the spatial volume of the integration and the infinitesimal volume element respectively. This equality's dependence on the operator under consideration disables universality. Hence, it is better to deal with the state vector whose elements are operators like positions and momenta, instead of this operator. We define the state vector denoted by \mathbf{s} as follows

$$\mathbf{s} \equiv [\widehat{s}_1 \dots \widehat{s}_n]^T \quad (2)$$

where n denotes the “system's dimension”. The state vector's Kronecker square (Kronecker product with itself) is given explicitly below

$$\mathbf{s}^{\otimes 2} \equiv \mathbf{s} \otimes \mathbf{s} \equiv [s_1 \mathbf{s}^T \dots s_n \mathbf{s}^T]^T. \quad (3)$$

This can be extended to the following general formula

$$\mathbf{s}^{\otimes m} \equiv \mathbf{s} \otimes \mathbf{s}^{\otimes(m-1)} \equiv [s_1 \mathbf{s}^{\otimes(m-1)T} \dots s_n \mathbf{s}^{\otimes(m-1)T}]^T, \quad m = 0, 1, 2, 3, \dots \quad (4)$$

where the m th Kronecker power of the state vector has n^m number of elements. The zeroth Kronecker power is defined as the universal scalar, just 1 (that is, it is a single element vector).

The state vector's expected value satisfies the following equation

$$\frac{d\langle\mathbf{s}\rangle(t)}{dt} = \left\langle \frac{i}{\hbar} [\widehat{H}\mathbf{s} - \mathbf{s}\widehat{H}] \right\rangle \quad (5)$$

We assume

$$\frac{i}{\hbar} [\widehat{H}\mathbf{s} - \mathbf{s}\widehat{H}] \equiv \sum_{j=0}^{\infty} \mathbf{H}_j \mathbf{s}^{\otimes j} \quad (6)$$

where \mathbf{H}_j is a rectangular matrix of $n \times n^j$ type. (5) can be extended to Kronecker powers by using certain properties of the Kronecker product together with the matrix product to get

$$\frac{d\langle \mathbf{s}^{\otimes j} \rangle(t)}{dt} = \sum_{\ell=0}^{\infty} \mathbf{E}_{j,\ell} \langle \mathbf{s}^{\otimes \ell} \rangle(t), \quad j = 0, 1, 2, \dots \tag{7}$$

where

$$\mathbf{E}_{j,\ell} \equiv \sum_{k=0}^{j-1} \mathbf{I}^{\otimes k} \otimes \mathbf{H}_{j-\ell+1} \otimes \mathbf{I}^{\otimes(j-1-k)} \tag{8}$$

where \mathbf{I} stands for the $n \times n$ identity matrix. If we define

$$\boldsymbol{\xi}(t) \equiv \left[\langle \mathbf{s}^{\otimes 0} \rangle(t)^T \quad \langle \mathbf{s}^{\otimes 1} \rangle(t)^T \quad \dots \right]^T, \quad \mathbf{E} \equiv \begin{bmatrix} \mathbf{E}_{0,0} & \dots & \mathbf{E}_{0,m} & \dots \\ \vdots & \ddots & \vdots & \dots \\ \mathbf{E}_{m,0} & \dots & \mathbf{E}_{m,m} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \tag{9}$$

then we obtain

$$\frac{d\boldsymbol{\xi}(t)}{dt} = \mathbf{E}\boldsymbol{\xi}(t) \tag{10}$$

which is an infinite set of ODEs whose coefficient matrix \mathbf{E} is composed of constant elements. The second block element of its solution gives the sought expected value of the state vector. The solution can be formally written as

$$\boldsymbol{\xi}(t) = e^{t\mathbf{E}}\boldsymbol{\xi}(0) \tag{11}$$

where

$$\boldsymbol{\xi}(0) \equiv \left[\langle \mathbf{s}^{\otimes 0} \rangle(0)^T \quad \langle \mathbf{s}^{\otimes 1} \rangle(0)^T \quad \dots \right]^T \tag{12}$$

and

$$\langle \mathbf{s}^{\otimes m} \rangle(0) \equiv \int_V dV \psi_0(\mathbf{x})^* \mathbf{s}^{\otimes m} \psi_0(\mathbf{x}), \quad m = 0, 1, 2, \dots \tag{13}$$

We find this information sufficient for our purposes here. Further details can be found in Demiralp’s paper which is the first part of this trilogy [5].

2 Evolution matrix spectral entities in the case of triangularity

If the system under consideration has a vanishing \mathbf{H}_0 at the expansion point then the evolution matrix becomes upper block triangular. This facilitates the spectral investigations very much since the block triangularity separates the infinite spectral problem

to infinite number of finite spectral problems. The spectral entities of each diagonal block should be evaluated to get all spectral entities of the evolution matrix.

Let us now reconsider (8) for $\ell = j$ and write

$$\mathbf{E}_{j,j} \equiv \sum_{k=0}^{j-1} \mathbf{E}_{j,j}^{(k)}, \quad j = 0, 1, 2, \dots \quad (14)$$

where

$$\mathbf{E}_{j,j}^{(k)} \equiv \mathbf{I}^{\otimes k} \otimes \mathbf{H}_1 \otimes \mathbf{I}^{\otimes (j-1-k)}, \quad k = 0, 1, 2, \dots, (j-1), \quad j = 0, 1, 2, \dots \quad (15)$$

A careful look at (15) reveals the following commutativity relation.

$$\mathbf{E}_{j,j}^{(k)} \mathbf{E}_{j,j}^{(\ell)} = \mathbf{E}_{j,j}^{(\ell)} \mathbf{E}_{j,j}^{(k)}, \quad k, \ell = 0, 1, 2, \dots, (j-1) \quad (16)$$

which means that the eigenvector sets of all these $n^j \times n^j$ type matrices should be the same. To proceed it is better to rewrite (15) in the following more explicit form

$$\mathbf{E}_{j,j}^{(k)} = \underbrace{\mathbf{I} \otimes \dots \otimes \mathbf{I}}_{k \text{ matrices}} \otimes \mathbf{H}_1 \otimes \underbrace{\mathbf{I} \otimes \dots \otimes \mathbf{I}}_{(j-k-1) \text{ matrices}}, \quad k = 0, 1, 2, \dots, (j-1), \quad j = 0, 1, 2, \dots \quad (17)$$

which explicitly shows that $\mathbf{E}_{j,j}^{(k)}$ is composed of j factors involving two commutative matrices, \mathbf{I} and \mathbf{H}_1 . Hence the eigenvectors of this matrix should be constructed from the eigenvectors of these two matrices. However, the identity matrix has a very specific nature such that all its eigenvalues are same and equal to 1. This leaves its eigenvectors arbitrary. Indeed any n element orthonormal set of vectors can be used as the eigenvectors of the identity matrix. On the other hand the eigenvectors of an n factor Kronecker product are all possible Kronecker product combinations of the factors' eigenvectors. All these mean that the eigenvectors of $\mathbf{E}_{j,j}^{(k)}$ should be all possible Kronecker products of the eigenvectors of the matrix \mathbf{H}_1 .

Let us now write the spectral problem of the matrix \mathbf{H}_1 as follows

$$\mathbf{H}_1 \mathbf{h}_j^{(r)} = h_j \mathbf{h}_j^{(r)}, \quad \mathbf{H}_1^T \mathbf{h}_j^{(\ell)} = h_j \mathbf{h}_j^{(\ell)}, \quad j = 1, 2, 3, \dots, n \quad (18)$$

where the eigenvector superscripts (r) and (ℓ) stand for the right and left eigenvectors respectively. Since \mathbf{H}_1 may not be symmetric, there is no warranty for the equality of the algebraic and geometric multiplicities of the multiple eigenvectors. The cases without this equality do not permit for the diagonalization of the matrix \mathbf{H}_1 . However it is possible to get Jordan canonical form. We however do not deal with these cases and assume that \mathbf{H}_1 is diagonalizable. It is not hard to extend what we will have under this assumption to the case of Jordan canonical forms.

Under diagonalizability conditions we can take the left and right eigenvectors of \mathbf{H}_1 mutually orthonormal. In other words

$$\mathbf{h}_j^{(\ell)T} \mathbf{h}_k^{(r)} = \delta_{j,k}, \quad j, k = 1, 2, 3, \dots, n \tag{19}$$

where δ denotes the Kronecker symbol.

If we now write the eigenvalue problem for $\mathbf{E}_{j,j}^{(k)}$ as follows

$$\begin{aligned} \mathbf{E}_{j,j}^{(k)} \mathbf{e}_{m_1, \dots, m_j}^{(j,k,r)} &= e_{m_1, \dots, m_j} \mathbf{e}_{m_1, \dots, m_j}^{(j,k,r)}, \\ \mathbf{E}_{j,j}^{(k)T} \mathbf{e}_{m_1, \dots, m_j}^{(j,k,\ell)} &= e_{m_1, \dots, m_j} \mathbf{e}_{m_1, \dots, m_j}^{(j,k,\ell)}, \\ j, k &= 1, 2, 3, \dots, n, \quad m_1, \dots, m_j = 1, 2, 3, \dots, n \end{aligned} \tag{20}$$

then we get

$$\begin{aligned} \mathbf{e}_{m_1, \dots, m_j}^{(j,k,r)} &= \mathbf{h}_{m_1}^{(r)} \otimes \dots \otimes \mathbf{h}_{m_j}^{(r)}, \\ \mathbf{e}_{m_1, \dots, m_j}^{(j,k,\ell)} &= \mathbf{h}_{m_1}^{(\ell)} \otimes \dots \otimes \mathbf{h}_{m_j}^{(\ell)}, \\ e_{m_1, \dots, m_j}^{(j,k)} &= h_{m_k} \end{aligned} \tag{21}$$

which can be extended to the matrix $\mathbf{E}_{j,j}$ by the following equalities

$$\begin{aligned} \mathbf{e}_{m_1, \dots, m_j}^{(j,r)} &= \mathbf{h}_{m_1}^{(r)} \otimes \dots \otimes \mathbf{h}_{m_j}^{(r)}, \\ \mathbf{e}_{m_1, \dots, m_j}^{(j,\ell)} &= \mathbf{h}_{m_1}^{(\ell)} \otimes \dots \otimes \mathbf{h}_{m_j}^{(\ell)}, \\ e_{m_1, \dots, m_j}^{(j)} &= h_{m_1} + \dots + h_{m_j} \end{aligned} \tag{22}$$

where

$$\begin{aligned} \mathbf{E}_{j,j} \mathbf{e}_{m_1, \dots, m_j}^{(j,r)} &= e_{m_1, \dots, m_j} \mathbf{e}_{m_1, \dots, m_j}^{(j,r)}, \\ \mathbf{E}_{j,j}^T \mathbf{e}_{m_1, \dots, m_j}^{(j,\ell)} &= e_{m_1, \dots, m_j} \mathbf{e}_{m_1, \dots, m_j}^{(j,\ell)}, \\ j, k &= 1, 2, 3, \dots, n, \quad m_1, \dots, m_j = 1, 2, 3, \dots, n. \end{aligned} \tag{23}$$

(22) shows that the eigenvectors of $\mathbf{E}_{j,j}$ are all the possible j -factor Kronecker products of the eigenvectors of \mathbf{H}_1 . We tend to use normalized eigenvectors for uniqueness. The eigenvalues of $\mathbf{E}_{j,j}$ are the j -term sums of the eigenvalues corresponding to the eigenvector in the relevant Kronecker product.

When j is greater than n then some of the eigenvalues h_{m_k} s should be repeated. Hence the true and more simplified eigenvalue equation is as follows

$$e_{m_1, \dots, m_j}^{(j)} = m_1 h_1 + \dots + m_n h_n, \quad m_1 + \dots + m_n = n^j, \quad j > n \tag{24}$$

Therefore the eigenvalues of the evolution matrix are all possible linear combinations of the eigenvalues of \mathbf{H}_1 with natural number linear combination coefficients. The

eigenvalues of \mathbf{H}_1 need not be real entities. They may be complex or pure imaginary numbers as well. As a matter of fact, in the case of quantum mechanical systems pure imaginary eigenvalues are mostly encountered as long as no scattering cases are considered. Even zero eigenvalue may appear in certain circumstances. Imaginary eigenvalues should appear as complex conjugate pairs because of the real-valuedness of the matrix elements of \mathbf{H}_1 . This means that there should be infinite number of zero eigenvalues of the evolution matrix. We focus on this issue in the next section.

3 Zero eigenvalues of the evolution matrix

The zero eigenvalues of the evolution matrix, if they come from the structure of the matrix \mathbf{H}_1 (there is a single zero eigenvalue coming from the zero value of $\mathbf{E}_{0,0}$, this is however exceptional), then they should be infinitely many. This means the existence of an infinite number of corresponding eigenvectors of the evolution matrix at the same time. These eigenvectors span an infinite subspace in infinite dimensional Cartesian space under consideration. If the initial expected value vector $\xi(0)$ lies in this subspace then the time variation (first temporal derivative) of the vector $\xi(t)$ vanishes for all time instances. This implies that $\xi(t)$ remains constant for all time instances. However this can happen only when the system's Hamiltonian is time independent, autonomous in mathematical language. On the other hand the subspace of evolution matrix eigenvectors corresponding to zero eigenvalues coming from \mathbf{H}_1 is spanned by quite specific initial expected value vectors which can only be produced by choosing the wave function specifically. In fact, the wave functions which are the eigenfunctions of the Hamiltonian operator produce such eigenvectors of zero eigenvalues. Hence the solution of the zero eigenvalue problem of the evolution matrix corresponds to the solution of the eigenvalues and eigenfunctions of the Schrödinger operator. While the latter is a PDE solving problem the former is completely algebraic. On the other hand passing from one of these two type problems to the other has not been carefully investigated in a detailed manner and will be at focus in our close future works.

4 Suppressing the norms via redefinition of the state vector

As we have investigated in the first part [5] of this trilogy the mathematical fluctuation theory [6–22] helps to get stable truncated approximant sequences. Even though we have not stated there, this may however show temporary stabilities because of the increasing tendency of the Kronecker power expectation values of the state vector. This especially happens when one or more of the system vector operators are unbounded. Unboundedness somehow sucks most of the converging capability of the Fluctuationlessness Theorem. This urges us to convert the unbounded system vector elements to bounded ones through appropriate transformations. To this end we may assume that \hat{s}_j , the state vector element which is an operator, is unbounded like the momentum operator or the position operators in semi infinite or infinite geometries. Then we may replace it with the new operator \hat{s}'_j as follows

$$\hat{s}'_j \equiv \left[1 + \hat{s}_j^2 \right]^{-1} \left(\alpha_0 + \alpha_1 \hat{s}_j + \alpha_2 \hat{s}_j^2 \right) \quad (25)$$

where the operator \widehat{s}_j is assumed to be Hermitian and therefore the right hand side expression is bounded, and, the α parameters can be chosen depending on the needs. So the newly formed state vector including \widehat{s}'_j instead of \widehat{s}_j becomes bounded for this element. If all elements are made bounded in a similar fashion then the Fluctuationlessness Theorem can be efficiently used.

5 Singularities in the Hamiltonian

The probabilistic evolution philosophy is based on the inspiration from the analyticity and therefore Taylor series. However this inspiration remains applicable only when the system's Hamiltonian has no singularities. Since the Hamiltonian's dependence on the momenta is rather multinomial (conical in fact) its position dependent part, that is, the potential gains a lot of importance for the singularities. If the potential function has singularities somewhere in the complex plane of the spatial variables then it affects the solution of the Schrödinger equation and therefore the expected values. This means that (6) remains no longer valid. It must be replaced by something different. In the case of polar singularities Taylor series are replaced by Laurent series which has inverse powers of the independent variable or its deviation from a fixed reference point, together with the nonnegative powers. This may inspire us to introduce the inverse Kronecker powers of the state operators. However these powers are undefined and, if we enforce to get a definition, are faced with certain inconsistencies. On the other hand we have extended the state vector by adding certain elements which are reciprocals of certain elements to use probabilistic evolution approach (PEA) on the ODEs whose descriptive functions do not have Taylor series but Laurent series. So the same thing can be done here. If the inverses of the operator \widehat{s}_j appear in the Hamiltonian's series representation then we can define a state vector as follows

$$s' \equiv \begin{bmatrix} \widehat{s}_1 \\ \vdots \\ \widehat{s}_n \\ \widehat{s}_j^{-1} \end{bmatrix} \tag{26}$$

This facilitates the analysis if the singularities come from the reciprocal of a single variable. If there appear more than one reciprocals then all corresponding reciprocals should be added to the state vector. This apparently increases the dimension of the space. Hence, in this sense, taking care of the singularities is a matter of appropriate space extension. The reciprocals of the independent state operators may not be the only agents causing singularities. Instead, certain expressions concerning state operators may appear as the major causes of the singularities. Then those terms should be appropriately involved in an augmented state vector. If those operators remain inside a set which is closed under the operation taking the commutator with the system Hamiltonian then augmentations of this type work and the space extension solves the singularity problem. Otherwise certain precautions should be taken.

The addition of the reciprocals or singular expressions to the state vector may prevent the expectation value evaluation unless very specific initial wave functions are

taken into consideration. To relax this limitation what we can do is to enter weight operators for removing the nonintegrability of singular structures. This issue is under an intense study and we report the results as soon as satisfactory structures are constructed.

6 Getting conicality via space extension

Space extension [3,4,23,24] is an approach which is used in different forms and for different purposes. The main theme of the approach is to add more unknowns or components to the entities controlling or defining the system under consideration. Here we use it to get conicality for a specifically given quantum system.

Consider the following quantum quartic anharmonic oscillator

$$\widehat{H} \equiv \frac{1}{2\mu}\widehat{p}^2 + \frac{\kappa_1}{2}\widehat{q}^2 + \frac{\kappa_2}{4}\widehat{q}^4 \quad (27)$$

where μ denotes the mass of the oscillator while κ_1 and κ_2 stand for the elastic force constant and anharmonicity constant respectively. The system is a physically one dimensional particle and is determined by the momentum and position operators respectively. That is

$$\mathbf{s} \equiv \begin{bmatrix} \widehat{p} \\ \widehat{q} \end{bmatrix} \quad (28)$$

whose Kronecker square is explicitly given below to show the structuring

$$\mathbf{s}^{\otimes 2} \equiv \begin{bmatrix} \widehat{p}^2 \\ \widehat{p}\widehat{q} \\ \widehat{q}\widehat{p} \\ \widehat{q}^2 \end{bmatrix} \quad (29)$$

The commutator of the system Hamiltonian with the state vector is given below

$$\frac{i}{\hbar} [\widehat{H}\mathbf{s} - \mathbf{s}\widehat{H}] = \mathbf{H}_1\mathbf{s} + \mathbf{H}_3\mathbf{s}^{\otimes 3} \quad (30)$$

where

$$\mathbf{H}_1 \equiv \begin{bmatrix} 0 & -\kappa_1 \\ \frac{1}{\mu} & 0 \end{bmatrix} \quad (31)$$

$$\mathbf{H}_3 \equiv \begin{bmatrix} 0 & -\kappa_1 & 0 & 0 & 0 & 0 & 0 & -\kappa_2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (32)$$

This system's evolution matrix has only two nonzero diagonals which are the main diagonal and its second nearest upper neighbor. Apparently triangularity exists and the

matrix \mathbf{H}_1 has two pure imaginary eigenvalues, $\pm i\sqrt{\kappa/\mu}$ which are complex conjugates. Hence their sum vanish. There are infinitely many couple of eigenvalues in the spectrum of the evolution matrix. Hence the zero spectrum (infinitely multiple zeroes) is not empty and corresponds to the eigenenergies and corresponding eigenfunctions of the relevant Schrödinger equation.

Despite the two band structure, there is no conicality but third degree multinomiality in the evolution matrix. To get conicality we can use the space extension. To this end we can define the following augmented state vector

$$\mathbf{s}_{aug} \equiv \begin{bmatrix} \hat{p} \\ \hat{q} \\ \hat{q}^2 \end{bmatrix} \tag{33}$$

which produces

$$\frac{i}{\hbar} [\hat{H}\mathbf{s}_{aug} - \mathbf{s}_{aug}\hat{H}] = \mathbf{H}_1\mathbf{s}_{aug} + \mathbf{H}_2\mathbf{s}_{aug}^{\otimes 2} \tag{34}$$

where

$$\mathbf{H}_1 \equiv \begin{bmatrix} 0 & -\kappa_1 & 0 \\ \frac{1}{\mu} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{35}$$

and

$$\mathbf{H}_2 \equiv \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\kappa_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\mu} & 0 & \frac{1}{\mu} & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{36}$$

where the matrix \mathbf{H}_1 has again the same eigenvalues together with an additional zero eigenvalue. Apparently conicality exists in this structure.

7 Conclusion

We have focused certain secondary but very important issues in this second part of the trilogy on probabilistic evolution approach. We have given a specific importance on the spectral properties of the evolution matrix. As a preliminary step we have mentioned the relation between the zero spectrum (infinitely many zero eigenvalues) of the evolution matrix and the eigenvalue problem of the Hamilton operator (time independent Schrödinger equation). In this direction there is abundancy of applications from practical systems for future works. We have also discussed how to take care of singularities and found that the space extension stands as a good tool to this end although there is no complete theory yet. The space extension can also be used to get multinomiality or conicality. A rather simple system of quartic quantum anharmonic oscillator is taken as the target for the illustrative application. The last resources

[25–29] in the reference list are about the ODEs for giving an idea about the recent developments even though we do not need these methods for solving probabilistic evolution equations.

The final part of this trilogy is devoted to an introductory investigation of the Liouville systems.

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