Quantum Mechanical Matrix Ordinary Differential Equations and Their Solutions by Characteristic Evolutions

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Abstract: In this work we show that a large class of second order matrix ordinary differential equations can be solved with the aid of an appropriate linear matrix ordinary differential equation whose solutions describe a motion we call “Characteristic Evolutions” as long as the accompanying initial conditions on the unknowns and their first derivatives possess some specific properties. The linear equations describing characteristic evolutions have a specific operator we call Hamiltonian which may have time variance depending on the structure of the matrix ODEs under consideration. In the derivation and utilization of what we obtain, recently developed “Fluctuation Free Matrix Representation” approximation is also used. Certain illustrative implementations for pretty simple cases where analytic solutions can be obtained are also given.

Key–Words: Matrix ODEs, Quantum mechanics, Expectation Value, Fluctuation Free Matrix Representation.

1 Introduction
The following matrix ordinary differential equation will be kept on the focus in this work
\[ \ddot{Z}(t) = f(Z(t), t) \] (1)
which is accompanied by the initial conditions
\[ Z(0) = A, \quad \dot{Z}(0) = B \] (2)
where the initially given matrices A and B are assumed to be Hermitian, that is,
\[ A^\dagger = A, \quad B^\dagger = B, \] (3)
and they also satisfy
\[ B^T = -B, \quad AB - BA = iI, \] (4)
In this formulae Z(t) denotes a time variant \( n \times n \) type matrix while f stands for a bivariate function which is assumed to have certain analyticity features allowing us to use fluctuation free matrix representation concept. The symbol \( \dagger \) corresponds to the Hermitian conjugation while I denotes the \( n \times n \) unit matrix.

The above type of matrix ordinary differential equations (MODEs) becomes a nonlinear equation unless the function f defines an affine transformation at every time instant. It is possible to produce analytic solution for the case of linearity. However, the nonlinear cases may create many difficulties which can not be handled with the tools and the concepts of the linear vector spaces at the first glance. Hence, it becomes very important to find even an indirect way of solving these equations by using again linear vector space concepts and tools. Fortunately this happens to exist and we can develop a method to solve these equations in such a way that some linear MODEs can be constructed to express the solution of the MODE given by (1) and related following conditions above. This paper involves all details of this procedure.

The paper is organized as follows. The second section explains how the solutions can be constructed to the MODE in (1). The third section deals with the Hamiltonian matrix mentioned above. The fourth section presents an illustrative application of what we construct here. The fifth section which contains the concluding remarks finalizes the paper.

2 Solution via Characteristic Evolution
Let us seek a solution in the following structure for Z(t) appearing in (1)
\[ Z(t) \equiv T(t)^\dagger AT(t) \] (5)
which enforces T to satisfy
\[ T(0) = I \] (6)
(5) defines the time variance in Z(t) through the matrix T(t) which is responsible for all variations with
respect to time, \( t \) and it brings the nonlinearity to the unknown because it appears twice as itself and as its Hermitian conjugate in the product structure assumed for the unknown matrix \( Z(t) \). This recalls the quantum evolutions where an operator evolving in time is related to its value at the beginning of the evolution via an expression same as the one in (5) with one exception that the entity called time evolution operator takes the place of the matrix \( T(t) \). This inspires us to treat the matrix \( T(t) \) as if it is somehow an evolution operator and urges us to write the following equation which is corresponding to the time dependent Schrödinger equation of Quantum Mechanics and describes the evolution characterized by \( Z(t) \).

\[
\dot{Z}(t) = -iH(t)Z(t)
\]

(7)

where \( i \) is the imaginary unit number and \( H(t) \) stands for a real symmetric \( n \times n \) type unknown matrix which is undetermined yet. The Hermitian conjugation of the both sides in (7) produces

\[
\dot{Z}(t) = -iH(t)Z(t) = -iH(t)\dot{Z}(t)
\]

(8)

Premultiplication of (7) by \( T(t) \) and postmultiplication of (8) by \( T(t) \) and then the addition of the resulting equations side by side produces

\[
\frac{d}{dt} \left[ T(t)^\dagger T(t) \right] = 0
\]

(9)

and, via the above initial condition for \( T(t) \), we get

\[
T(t)^\dagger T(t) = I
\]

(10)

This result shows that the Hermitian conjugate of the matrix \( T(t) \) is equivalent to its inverse. Therefore it is a unitary matrix. The time evolution operators of the quantum mechanics are also unitary. Hence the differential equation satisfied by \( T(t) \) provides \( T(t) \) with this property because of the Hermiticity in the matrix \( H(t) \).

Now a careful investigation shows that

\[
\dot{Z}(t) = T(t)^\dagger \left\{ i [ H(t)A - AH(t) ] \right\} T(t) = -iT(t)^\dagger [ H(t), A ] T(t)
\]

(11)

where the symbol \( [ A_1, A_2 ] \) stands for the commutator of any two square matrices with same dimension (it is \( n \) here), denoted by \( A_1 \) and \( A_2 \). Its explicit definition is given below

\[
[A_1, A_2] \equiv A_1A_2 - A_2A_1
\]

(12)

Now by differentiating the both sides of (11) in time and using the analysis to get (11) we can obtain the following equality

\[
\dot{Z}(t) = -T(t)^\dagger [ H(t), [ H(t), A ] ] T(t), \quad \text{which means}
\]

\[
\dot{Z}(0) = \tilde{A}(0) = B
\]

(13)
or more explicitly
\[ i \left[ H(0) A - AH(0) \right] = B. \] (23)

We can write the following algebraic equalities
\[ i \left[ \frac{1}{2} B^2 A - \frac{1}{2} A B^2 \right] = -\frac{i}{2} B (A B - B A) \]
\[ -\frac{i}{2} (A B - B A) B = B \] (24)

where we have used the second property of (4). A careful investigation shows that
\[ i \left[ g (A, t) A - A g (A, t) \right] = 0 \] (25)
holds for any bivariate function \( g \) which is analytic in its first argument’s complex plane for a region involving the spectrum of \( A \) as an interior region. All these mean that we can propose the following structure for the matrix \( H(t) \)
\[ H(t) = \frac{1}{2} B^2 + g (A, t) \] (26)
which leaves us with the task of determining the unknown bivariate function \( g (A, t) \). To this goal we can write first
\[ \tilde{A}(t) = B \] (27)
which can be obtained rather easily and then get the following equation from (20)
\[ i \left[ H(t), B \right] = f (A, t) \] (28)
or
\[ i \left[ g (A, t), B \right] = f (A, t) \] (29)
which has been obtained by using the fact that the square of any square matrix commutes with itself.

To solve the algebraic equation in (29) for \( g (A, t) \) we can use \( g(z, t) \)'s Taylor series expansion at a point \( z_g \) which is chosen such that \( g(z, t) \) is analytic in a disk, centered at that point, with radius sufficing to cover the spectrum of the matrix \( A \) in that disk. That is,
\[ g(z, t) = \sum_{k=0}^{\infty} g_k (z_g, t) (z - z_g)^k \] (30)
where the expansion coefficient, \( g_k (z_g, t) \) is the the value of the \( g(z, t) \)'s \( k \)th \( z \)-derivative evaluated at \( z = z_g \) divided by \( k! \). This expansion enables us to write
\[ g (A, t) = \sum_{k=0}^{\infty} g_k (z_g, t) (A - z_g I)^k \] (31)

and therefore
\[ i \left[ g (A, t), B \right] = \sum_{k=0}^{\infty} g_k (z_g, t) \left[ (A - z_g I)^k, B \right]. \] (32)

Now we can write
\[ i \left[ (A - z_g I)^0, B \right] = i \left[ I, B \right] = 0 \] (33)
\[ i \left[ (A - z_g I)^1, B \right] = i \left[ A, B \right] = -I \] (34)
\[ i \left[ (A - z_g I)^2, B \right] = \ldots \] (35)
where we have used the second property in (4). These equalities urges us to conjecture
\[ i \left[ (A - z_g I)^k, B \right] = -k (A - z_g I)^{k-1}, \]
\[ k = 0, 1, 2, \ldots \] (36)

For proof we assume the validity of this formula for an arbitrary positive integer value \( k \) and then try to show its validity for \( k + 1 \). We can start to proceed as follows
\[ i \left[ (A - z_g I)^{k+1}, B \right] = i (A - z_g I)^k \left[ (A - z_g I) B - B (A - z_g I) \right] + i \left[ (A - z_g I)^k B - B (A - z_g I)^k \right] (A - z_g I) \] (37)
where we can use (34) and (36) which assumed to be valid above to get
\[ i \left[ (A - z_g I)^{k+1}, B \right] = -(k + 1) (A - z_g I)^k, \]
\[ k = 0, 1, 2, \ldots \] (38)
which completes the validity proof of (36) in accordance with the mathematical induction.

Now the use of (36) in (32) gives
\[ i \left[ g (A, t), B \right] = \sum_{k=0}^{\infty} k g_k (z_g, t) (A - z_g I)^{k-1} \] (39)
where

\[ g_z(z,t) = \sum_{k=0}^{\infty} kg_k(z) (z - z_g)^{k-1} \]

which is analytic in the same domain of \( g(z,t) \). All these mean

\[ -g_z(z,t) = f(z,t) \]

and therefore

\[ g(z,t) = \int_{z_g}^{z} d\zeta f(\zeta, t) \]

which urges us to take \( z_g = z_f \) to get overlapping analyticity regions for \( f(z,t) \) and \( g(z,t) \). The arbitrary integration constant appearing in the derivation of (43) has been selected in such a way that \( g(z,t) \) vanishes at the center of \( f(z,t) \)’s and therefore its analyticity disk. However, it can be chosen anything else without changing the analysis and the uniqueness of the solution since the difference coming from the different selections of this constant appears to be an exponential matrix factor whose argument is proportional to unit matrix in the definition of the matrix \( T(t) \) and is spontaneously cancelled out between the factors \( T(t) \) and \( T(t)^{\dagger} \).

Now we have completed the construction of the solution for (1). The structure of the matrix \( H(t) \) recalls the matrix representation of the Hamiltonian operator over a finite dimensional subspace of the Hilbert space of univariate functions which are analytic and therefore square integrable over a specified interval. Although there is no matrix representation and basis function here the structure of \( H(t) \) urges us to call it “Hamiltonian Matrix” of the system characterized by (1). The components of \( \frac{1}{2}B^2 \) and \( g(A,t) \) can be considered as the “Kinetic Energy” and time variant “Potential Energy” term under the inspiration of the quantum mechanics whose position and momentum operators correspond to the matrices \( A \) and \( B \) respectively. In the framework of these considerations the function \( f(A,t) \) corresponds to the force field over the system characterized by (1).

### 3 Some Particular Cases

The Hamiltonian Matrix we have constructed in the analysis of the previous section may take specific analytic forms if the time evolution matrix \( T(t) \) shows specific analytic structures. This may happen when the system’s force field term has certain specific functional structures. We are going to return to this issue a little bit later. We want to emphasize on a very general but specific case where the functional structure of the time evolution matrix \( T(t) \) can be found analytically without regarding to the functional structure of the force field in position. This is the case where the force field depends on the position only. If it can be written just as \( f(Z(t)) \) then the potential term of the Hamiltonian matrix \( H(t) \) loses its explicit time dependence and can be written as \( g(A) \). This removes the time dependence of \( H(t) \) since we can write

\[ H(A,B) = \frac{1}{2}B^2 + g(A) \]

where we have shown the dependence of the Hamiltonian matrix on the position and momentum matrices, \( A \) and \( B \). (44) enables us to write time evolution matrix \( T(t) \) as follows

\[ T(t,A,B) = e^{-itH(A,B)} \]

which implies

\[ Z(t,A,B) = e^{itH(A,B)}Ae^{-itH(A,B)} \]

Of course, this structure may require more attention than one will pay by looking its innocence mathematics because of the exponential matrix. Serious convergence problems may be encountered depending on how the eigenvalues of the Hamiltonian matrix are distributed in its spectrum. We do not intend to get into the details of this issue here.

Now we consider the case where the force field is time independent and linear as follows

\[ f(Z(t)) = -kZ(t) \]

where \( k \) is a given constant. This urges us to write

\[ g(A) = \frac{k}{2}A^2 \]

where we have taken \( z_g = 0 \) because the force field’s structure is analytic in every finite region of its argument’s complex plane and hence permits us to choose the value of the Taylor series expansion point arbitrarily. (48) implies

\[ H(A,B) = \frac{1}{2}B^2 + \frac{k}{2}A^2 \]

which has the form of a one dimensional harmonic oscillator with a support at the origin. The derivatives
of the matrix $Z(t, A, B)$ with respect to $t$ can be expressed as follows

$$Z^{(j)}(t, A, B) = e^{itH}A_j e^{-itH},$$

where the core matrices $A_j$ ($j = 0, 1, 2, ...$) satisfy the following recursion as can be shown by simply differentiating the both sides of the above equality.

$$A_{j+1} = i \left[ HA_j - A_j H \right], \quad A_0 = A,$$

$$j = 0, 1, 2, ...$$

A careful investigation shows that the Hamiltonian matrix given by (49) satisfy the following relations

$$i \left[ HA - AH \right] = B,$$

$$i \left[ HB - BH \right] = -kA,$$

which imply

$$A_{2j} = (-k)^j A,$$

$$A_{2j+1} = (-k)^j B,$$

$$j = 0, 1, 2, ...$$

or in a single equality

$$A_j = \frac{1 + (-1)^j}{2} (-k)^j A + \frac{1 - (-1)^j}{2} (-k)^{j+1} B,$$

$$j = 0, 1, 2, ...$$

Now we can write

$$Z(t, A, B) = \sum_{j=0}^{\infty} \frac{t^j}{j!} A_j$$

It is not hard to get the following result we give without intermediate manipulation details by combining the last two equalities

$$Z(t, A, B) = \cos(\sqrt{k}t) A + \frac{sin(\sqrt{k}t)}{\sqrt{k}} B$$

On the other hand, (1) takes the following form for this case

$$\dot{Z}(t, A, B) = -kZ(t)$$

whose solution can be considered as

$$Z(t, A, B) = c_1(t) A + c_2(t) B$$

by being inspired from the linearity and the given initial conditions. Insertion of this form to (57) produces the following equations

$$\ddot{c}_1(t) = -kc_1(t), \quad c_1(0) = 1;$$

$$\ddot{c}_2(t) = -kc_2(t), \quad \dot{c}_2(0) = 1,$$

the utilization of whose solutions in (58) produces a solution for $Z(t, A, B)$ coinciding with the previously obtained one.

This completes the analysis for this case. We do not intend to focus on some other particular cases since we find this section sufficiently comprehensive for the explanation of the characteristic evolution approach we develop here.

## 4 Conclusion

Our main focus in this work has been the solution of the matrix ordinary differential equations belonging to a class where it is possible to imitate what we do when we attempt to solve the evolution problems of the quantum mechanics. The equations are second order and are accompanied by the initial conditions on the values of the unknown’s itself and its first derivative at the beginning of the time. These initial values are assumed to be possessing certain specific properties. We constructed a solution which is related to the initial value of the unknown at every time instant via a hermitian type unitary mapping whose evolution matrix is unknown. This matrix needs to satisfy a linear matrix ordinary differential equation whose coefficient matrix has been called Hamiltonian matrix because it has a great analogy to the Hamiltonian of the quantum mechanics. Hamiltonian needed to be determined in such a way that the insertion of these structures mentioned above satisfy the original equations and accompanying boundary conditions. When this is done, the kinetic energy part and the potential energy part of the hamiltonian matrix are revealed. What we have caught the fact that the initial value of the unknown matrix of the problem plays the role of the position coordinate while the initial value of the unknown matrix derivative behaves like momentum. The potential term of the Hamiltonian, time variant or invariant, depends on the position matrix only and the right hand side of the original equation somehow characterizes as if a force field. We have focused on two cases: (1) the time independent Hamiltonian having problems (2) the time variant Hamiltonian but first degree polynomial structure in the force field term. We could be able to show that this approach here produces the analytic solution of the problem, which can be found by some other means.
The implementation of this method in the cases where the analytic solution is not possible can be based on approximating the time evolution matrix. Although we have not dealt with this issue here we are continuing to study these issues intensely. The author's opinion is that the approach explained here seems to be a powerful candidate for being a widely used method in practical applications and to open new and vast horizons in the research of these kind topics.

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