Solving Initial Value Problems of Multivariable Parabolic Systems via Expectation Values: Probabilistic Evolution, Exactness and Approximants

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Abstract: There is an abundancy of systems characterized by parabolic PDEs in science and engineering, especially in chemistry and physics. These systems have a scalar variable, we generally call time, defining the evolution of the system under consideration. The governing equation(s) involves the unknown(s) and their first order partial derivative(s) with respect to this variable. Time variant Schrödinger equations where the unknown is the wavefunction which is responsible for the probability density for the system and Liouville equations for the statistical mechanics where the unknown is somehow responsible for a density in the systems' phase space (here we use the plurality since both case may differ from Hamiltonian to Hamiltonian). Certain PDE(s), depending on so-called spatial coordinates, govern the behavior of the system in these and similar cases even though the partial differential equation nature is not necessarily needed. Hence we give the following equation for more abstractioning

$$i\frac{\partial \psi(t)}{\partial t} = \widehat{\mathcal{L}}\psi(t) \tag{1}$$

where we call the unknown entity $\psi(t)$ "wavefunction" by following the quantum mechanical tradition despite $\psi(t)$ need not be a true function. It may be anything like vector, matrix, function, or, operator as long as it lies in an appropriately defined Hilbert space. In this sense it has the abstract meaning "vector" (but not necessarily a Cartesian vector). $\widehat{\mathcal{L}}$ stands for a linear operator (which is not necessarily a partial differential operator) mapping from the Hilbert space, where $\psi(t)$ lies, to the same space. Even though it is not explicitly shown here the system is characterized by certain operators we call "System

Operators" like the positions and momenta in the case of quantum mechanics. We denote these operators by $\widehat{s}_1$,...,$\widehat{s}_n$ or in a shorthand notation $\widehat{\mathbf{s}}$.

One way to solve the equation in (1) is to find the vector $\psi(t)$ which may be not so technically easy as its first glance appearence implies even when $\widehat{\mathcal{L}}$ does not explictly depend on t. This autonomy is not so much greater limitation since it can be provided for us even (1) is nonautonomous at the expense of extending the space spanned by $\psi(t)$ to a higher dimension. The second possibility is the utilization of the expectation values of the system operator $\widehat{\mathbf{s}}$ and its outer powers. This excludes the determination of $\psi(t)$ but necessitates the evaluation of the expectation values for all nonnegative outer powers of the state operator. A vector ODE is constructed for each outer power of the state vector by using (1). However, the action of the commutator with $\widehat{\mathcal{L}}$ on each outer power is required. By following the general property encountered in the traditional cases we represent these actions in terms of certain Taylor expansion in outer powers of the state operator. Thus we arrive at an infinite set of ODEs with an infinite constant coefficient matrix we call "Evolution Matrix". The formal solution of this set of ODEs can be obtained in terms of a time variant exponential matrix over the Evolution Matrix and the initial value vector. Talk focuses on certain details of these and some related issues.