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On a perturbation method for partial differential equations

Francisco M Fernández

CEQUINOR (Conicet), Departamento de Química,
Facultad de Ciencias Exactas, Universidad Nacional de la Plata,
Calle 47 y 115, Casilla de Correo 962,
1900 La Plata, Argentina

E-mail: framfer@isis.unlp.edu.ar

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Abstract

We show that a recently developed perturbation method for partial differential equations can be rewritten in the form of an interaction picture. In this way it is possible to compare this approach with others such as the standard perturbation theory and a straightforward temporal expansion of the evolution operator. We choose a simple, exactly solvable model as an illustrative example.

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1. Introduction

Recently Durand and Franck [1] proposed a perturbation method for the systematic solution of a certain type of partial differential equation, and applied it to diffusion problems. One advantage of that approach is that the perturbation series conserves probability term by term.

The purpose of this paper is to show that the method developed by Durand and Franck [1] can be rewritten in the form of an interaction picture, similar to that commonly used in quantum mechanics. We believe that this point of view may facilitate the understanding and further discussion of the approach, as well as its application to other problems of physical interest.

2. Interaction picture

For convenience we write the problem in a quite general form as

$$\frac{\partial u(t)}{\partial t} = \hat{\mathcal{L}}u(t) \tag{1}$$

where we only indicate the temporal dependence of the solution $u(t)$, which may depend on other variables as well. If the linear operator $\hat{\mathcal{L}}$ does not depend on time, the formal solution of equation (1) reads

$$u(t) = \exp(t\hat{\mathcal{L}})u(0) \tag{2}$$

where $u(0)$ is the initial condition.

We assume that there exists an operator $\hat{\mathcal{L}}_0$ that we can consider sufficiently close to $\hat{\mathcal{L}}$, and such that we can easily obtain

$$u_0(t) = \exp(t\hat{\mathcal{L}}_0)u(0). \tag{3}$$

Under such conditions we write the time evolution operator $\hat{U}(t) = \exp(t\hat{\mathcal{L}})$ in the form of an interaction picture as follows:

$$\hat{U}(t) = \hat{K}(t)\exp(t\hat{\mathcal{L}}_0) \tag{4}$$

where the evolution operator in the interaction picture $\hat{K}(t)$ satisfies the differential equation

$$\frac{\partial \hat{K}(t)}{\partial t} = \hat{\mathcal{L}}\hat{K} - \hat{K}\hat{\mathcal{L}}_0 \tag{5}$$

as the reader may easily verify. In order to solve this equation we expand $\hat{K}(t)$ in a Taylor series about $t = 0$:

$$\hat{K}(t) = \sum_{n=0}^{\infty} \hat{A}_n \qquad \hat{A}_n = t^n \hat{K}_n \tag{6}$$

where $\hat{K}_0 = \hat{K}(0) = \hat{1}$ is the identity operator.

Taking into account equations (2)–(4) and (6), we write the solution $u(t)$ as a series

$$u(t) = \sum_{n=0}^{\infty} u_n(t) \tag{7}$$

where $u_n(t) = \hat{A}_n u_0(t)$. By straightforward substitution of the Taylor expansion (6) into the differential equation (5) we easily prove that the operators $\hat{A}_n$ satisfy the recurrence relation

$$(n+1)\hat{A}_{n+1} = t(\hat{\mathcal{L}}\hat{A}_n - \hat{A}_n\hat{\mathcal{L}}_0). \tag{8}$$

If we apply both sides of equation (8) to $u_0(t)$, and take into account that

$$\frac{\partial u_n(t)}{\partial t} = \frac{n}{t}u_n(t) + \hat{A}_n\hat{\mathcal{L}}_0 u_0(t) \tag{9}$$

we easily arrive at the recurrence relation obtained by Durand and Franck [1]:

$$u_{n+1}(t) = \frac{1}{n+1}\left[n + t\left(\hat{\mathcal{L}} - \frac{\partial}{\partial t}\right)\right]u_n(t). \tag{10}$$

3. Perturbation theory

We believe that the present alternative derivation of the method of Durand and Franck puts it in a clearer perspective for subsequent development and improvement, in particular because the interaction picture is well known and widely applied in quantum mechanics. For example, we can compare the method of Durand and Franck [1] with the standard perturbation theory in which one writes the operator $\hat{\mathcal{L}}$ as $\hat{\mathcal{L}}_0 + \lambda\hat{\mathcal{L}}'$, where λ is a perturbation parameter. If we substitute the λ-power series

$$\hat{K}(t) = \sum_{n=0}^{\infty} \lambda^n \hat{k}_n \tag{11}$$

into equation (5), and solve the resulting expression for the coefficients $\hat{k}_n$, we easily obtain

$$\frac{\partial \hat{k}_n}{\partial t} = [\hat{\mathcal{L}}_0, \hat{k}_n] + \hat{k}_{n-1}\hat{\mathcal{L}}' \tag{12}$$

and

$$\hat{k}_n(t) = \int_0^t \exp[(t-s)\hat{\mathcal{L}}_0]\hat{k}_{n-1}\hat{\mathcal{L}}' \exp[(s-t)\hat{\mathcal{L}}_0]\,\mathrm{d}s. \tag{13}$$

We clearly realize that the application of equation (10) is easier than the application of equation (13) because the former does not require any integration at all. Moreover, the successive application of the operator $\hat{\mathcal{L}}$ in equation (10) is much more straightforward than the repeated transformation in equation (13) by means of the exponential operator $\exp[(t-s)\hat{\mathcal{L}}_0]$.

4. Examples

A general and rigorous discussion of the convergent properties of different approaches is beyond the scope of this article. However, we can draw useful hints by means of a solvable model; here we choose the linear operators to be proportional to the Pauli matrices:

$$\hat{\mathcal{L}}_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \hat{\mathcal{L}}' = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \hat{\mathcal{L}} = \hat{\mathcal{L}}_0 + \lambda\hat{\mathcal{L}}'. \tag{14}$$

Taking into account the well known expression of the exponential function of a matrix, we easily obtain [2]

$$\hat{K}(t) = \begin{pmatrix} [\cosh(at) + \frac{\sinh(at)}{a}]\exp(-t) & \lambda\frac{\sinh(at)}{a}\exp(t) \\ \lambda\frac{\sinh(at)}{a}\exp(-t) & [\cosh(at) - \frac{\sinh(at)}{a}]\exp(t) \end{pmatrix} \tag{15}$$

where $a = \sqrt{1+\lambda^2}$. By simple inspection we realize that the matrix $\hat{K}(t)$ is singular at $\lambda = \pm\mathrm{i}$, whereas it is an entire function of t. In other words, the series (7) converges for all values of λ and t, while, on the other hand, the series (11) converges only for $|\lambda| < 1$ disregarding the value of t.

As a further test of the method of Durand and Franck we have compared it with the straightforward temporal expansion of the evolution operator for the simple model just outlined:

$$\hat{U}(t) = \begin{pmatrix} \cosh(at) + \frac{\sinh(at)}{a} & \lambda\frac{\sinh(at)}{a} \\ \lambda\frac{\sinh(at)}{a} & \cosh(at) - \frac{\sinh(at)}{a} \end{pmatrix} = \sum_{n=0}^{\infty} t^n \hat{U}_n. \tag{16}$$

By means of Maple we have calculated all the necessary matrix elements of the coefficients $\hat{U}_n$, constructed both approximate evolution matrices, and compared them with the exact one (16) for $a = 1.1$ and $a = 1.5$. In both cases we have arbitrarily chosen partial sums of degree 10 for the diagonal elements and 11 for the off-diagonal ones. We have found that the straightforward temporal expansion (16) gives better results for most matrix elements, which suggests that the method of Durand and Franck may not be the best choice for all time-evolution problems. This conclusion does not contradict the fact that such a method has proved to give accurate results in the case of diffusion [1]. Notice, for example, that if the initial probability distribution is given by a Dirac delta function, the application of $\exp(t\hat{\mathcal{L}}_0)$ produces a Gaussian function that is sufficiently well behaved for the subsequent application of equation (10), with the additional advantage mentioned earlier that the resulting series conserves probability at any order of approximation [1]. At first sight the straightforward expansion appears to be unsuitable for that problem.

5. Further comments

Finally, we would like to mention that since the rate of convergence of the series (7) increases as t decreases, an interesting alternative method for difficult cases consists of propagating the solution according to

$$u(t+\Delta t) = \hat{U}(\Delta t)u(t) \tag{17}$$

and expanding $\hat{K}(\Delta t)$ in a Taylor series (6) for a sufficiently small value of the temporal increment Δt.

References

[1] Durand R V and Franck C 1999 *J. Phys. A: Math. Gen.* **32** 4955
[2] Fernández F M and Castro E A 1996 *Algebraic Methods in Quantum Chemistry and Physics* (Boca Raton, FL: Chemical Rubber Company) appendix A