Unitary transformations depending on a small parameter

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Quantum Mechanics (QM) presented since its very creation a view of physical phenomena radically different to that of Classical Mechanics (CM). In many ways, however, CM played a seminal and guiding role in the construction of the quantum formalism. This is evident in the contributions of some of the founding fathers of QM: for example in the famous "Drei männer arbeit" by Born, Heisenberg and Jordan [1] in which they built the quantum perturbation theory in strong analogy with the classical version. In addition, all three of them were able to make use of their through knowledge of the classical theory, especially of the perturbation schemes and the theory of canonical transformations, for extending their matrix scheme to general quantum systems.

Since then the mutual relationship between QM and CM has been fruitful, manyfold and has gone in both ways. A fact that is not always sufficiently emphasized. One of the reasons is that once QM was formulated in Hilbert space the essentially linear character of the formalism made more evident the use of algebraic techniques in this context than in CM. Perturbation theory is another area in which one can say that the quantum treatment is more popular than its classical counterpart. Here again the underlying linear structure of the quantum case allows for a simpler presentation. This is especially true if one adheres to the old-fashioned formulation of classical canonical perturbation theory with mixed (new and old) coordinates in phase space. However, since the late 60's there is a clear alternative to this procedure. It arose in Celestial Mechanics [2] and found early applications in plasma physics and accelerator studies. This approach is based on the use of Lie algebraic methods in CM and originates a perturbation theory that, while being equivalent to the classical Poincaré–Von Zeipel's, is simpler in presentation and richer in applications.

In this presentation we adapt the Lie–Deprit algorithm of classical mechanics as a perturbation theory for general quantum systems. This approach has the advantage that it allows a unifying view, in the following sense. On one hand, it establishes a direct connection between the classical and the quantum formalism. On the other hand, the same algorithm can be applied both to time-independent and time-dependent quantum systems. In addition, and contrarily to the usual time dependent perturbation theory, the scheme is unitary at any order of approximation.

Suppose we are interested in a quantum system which can be described by a time independent Hamiltonian H_0 perturbed by a time-dependent $H'(t,\epsilon)$ that depends on a small parameter ϵ in such a way that $H'(t,\epsilon=0)=0$. The Hamiltonian whose dynamics has to be solved reads then

$$H(t,\epsilon) = H_0 + H'(t,\epsilon) \equiv H_0 + \sum_{n=1}^{\infty} \epsilon^n H_n(t), \tag{1}$$

where we have assumed that $H'(t,\epsilon)$ is analytic in ϵ. The time evolution of the wave function $\Psi(t)$ may be described in terms of the evolution operator, $\Psi(t) = U(t,t_0)\Psi(t_0)$, which is unitary and obeys the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}U(t,t_0) = H(t)U(t,t_0), \quad U(t_0,t_0) = I. \tag{2}$$

Since the dynamics corresponding to H_0 has been solved, one has $U_{H_0}(t,t_0) = \exp(-i(t-t_0)H_0/\hbar)$. The goal is then to construct a unitary near-identity transformation $T(t,\epsilon)$ such that the transformed system

$$i\hbar\frac{\partial}{\partial t}U_K(t,t_0) = K(t,\epsilon)U_K(t,t_0), \qquad U_K(t_0,t_0) = I \tag{3}$$

is easier to solve than the original equation (2). Then it is easy to verify that $U(t,t_0)$ is factorized as

$$U(t,t_0) = T(t,\epsilon)U_K(t,t_0)T^\dagger(t_0,\epsilon), \tag{4}$$

and the new Hamiltonian K is given by

$$K(t,\epsilon) = T^\dagger(t,\epsilon)H(t,\epsilon)T(t,\epsilon) + i\hbar\frac{\partial T^\dagger(t,\epsilon)}{\partial t}T(t,\epsilon). \tag{5}$$

Vey often we will take $T(t_0 = 0,\epsilon) = I$ in (4). We guarantee that T is indeed unitary is by introducing a skew-Hermitian operator $L(t,\epsilon)$ such that $T(t,\epsilon)$ is the solution of the operator differential equation $\frac{\partial}{\partial\epsilon}T(t,\epsilon) = -T(t,\epsilon)L(t,\epsilon)$. Equivalently,

$$\frac{\partial}{\partial\epsilon}T^\dagger(t,\epsilon) = L(t,\epsilon)\,T^\dagger(t,\epsilon), \qquad T^\dagger(t,0) = I. \tag{6}$$

The formal solution of this equation can be obtained by applying the so-called Magnus expansion [3], so that we can write $T^\dagger(t,\epsilon) = \exp(\Omega(t,\epsilon))$, where Ω is a skew-Hermitian operator. Deriving equation (5) with respect to ϵ we arrive after some algebra at

$$\frac{\partial K}{\partial\epsilon} = [L,K] + \mathrm{e}^{\mathrm{ad}_\Omega}\frac{\partial H}{\partial\epsilon} + i\hbar\frac{\partial L}{\partial t}, \tag{7}$$

where $[L,K] \equiv LK - KL$ and $\mathrm{ad}_\Omega B \equiv [\Omega, B]$, with $\mathrm{ad}^n_\Omega B \equiv \mathrm{ad}^{n-1}_\Omega B$.

At this stage, three different issues have to be addressed:

(1) Choose the new Hamiltonian K such that equation (3) is easy to solve.
(2) Compute the skew-Hermitian generator L of the required transformation.
(3) Construct the unitary transformation T from the generator L, or equivalently, the operator Ω in $T = \exp(-\Omega)$.

It turns out that first two problems above enumerated can be solved perturbatively with equation (7), whereas the third can be treated independently. To proceed, we introduce in addition to (1), the following series expansions:

$$K(t,\epsilon) = \sum_{n=0}^{\infty}\epsilon^n K_n(t), \qquad L(t,\epsilon) = \sum_{n=0}^{\infty}\epsilon^n L_{n+1}(t). \tag{8}$$

Then, by applying the Magnus expansion, it is possible to determine $\Omega(t,\epsilon)$ as a power series in ϵ, $\Omega(t,\epsilon)=\sum_{n=1}^{\infty}\epsilon^n v_n(t)$ and the $v_n(t)$ can be expressed in terms of $L_j(t)$. In particular

$$v_1 = L_1, \quad v_2 = \frac{1}{2}L_2, \quad v_3 = \frac{1}{3}L_3 - \frac{1}{12}[L_1, L_2].$$

On the other hand, we have $\mathrm{e}^{\mathrm{ad}_\Omega}\frac{\partial H}{\partial \epsilon} = \sum_{n=0}^{\infty}\epsilon^n w_n(t)$ which can also be obtained algorithmically, its first terms being

$$w_0 = H_1, \;\; w_1 = 2H_2 + [L_1, H_1], \;\; w_2 = 3H_3 + 2[L_1, H_2] + \frac{1}{2}[L_2, H_1] + \frac{1}{2}[L_1, [L_1, H_1]].$$

Finally, inserting these series into (7) and collecting terms of the same power in ϵ, results in the following homological equation

$$i\hbar\frac{\partial L_n}{\partial t} + [L_n, H_0] = nK_n - \tilde{F}_n, \qquad n = 1, 2, \ldots \tag{9}$$

with

$$\tilde{F}_n = \sum_{j=1}^{n-1}[L_{n-j}, K_j] + w_{n-1} \tag{10}$$

in addition to $K_0 = H_0$. This equation admits the formal solution ($L_n(t_0 = 0) = 0$)

$$L_n(t) = -\frac{i}{\hbar}\int_0^t \mathrm{d}u\, \mathrm{e}^{-i(t-u)H_0/\hbar}\big(nK_n(u) - \tilde{F}_n(u)\big)\, \mathrm{e}^{i(t-u)H_0/\hbar}. \tag{11}$$

The election of a particular K is a degree of freedom of the method, and thus it can be adapted to any particular problem one is dealing with. Perhaps the simplest option is to take $K = H_0$ or equivalently $K_n = 0$ for $n \geq 1$. In this way one tries to construct a unitary transformation in such a way that in the new image there is no perturbation at all. In that case $U_K(t) = \exp\big(-iH_0(t-t_0)/\hbar\big)$ and

$$U(t) = T(t,\epsilon)\, \mathrm{e}^{-\frac{i}{\hbar}H_0(t-t_0)} = \mathrm{e}^{-\Omega(t,\epsilon)}\, \mathrm{e}^{-\frac{i}{\hbar}H_0(t-t_0)}. \tag{12}$$

Other options are of course valid. For instance, if H_0 has a pure non-degenerate point spectrum we can choose K_n diagonal. This is the natural choice when the original Hamiltonian (1) is time independent. It is also worth stressing that this procedure can be generalized to *any* linear differential equation and thus constitutes a novel approach to carry out perturbative analysis whereas preserving qualitative (geometric) properties of the exact solution.

References

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[3] W. Magnus, *On the exponential solution of differential equations for a linear operator*, Commun. Pure Appl. Math. **7** (1954), 649–673.