Time-Dependent Perturbation Theory with a Classical Limit

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We construct a quantum mechanical perturbation theory which uses the multiple time scale technique. Working with the time translation operator, we use a variant on the method of Bender and Bettencourt. Our perturbation theory smoothly crosses over to the classical result as $\hbar \to 0$. It is seen that this technique has a nonperturbative element built into it.

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In classical dynamics, one of the best known techniques for handling nonlinear systems is the Poincaré-Lindstedt perturbation theory. What would be its quantum mechanical generalization? This is not straightforward because the Poincaré-Lindstedt technique is predicated on the fact that the dynamics is periodic while the quantum dynamics of the expectation value of an observable is, in general, quasiperiodic. This is true, e.g, for the expectation value of the position operator x of an anharmonic oscillator governed by the Hamiltonian

$$H = p^2/2m + 1/2m\omega^2 x^2 + 1/4\lambda x^4. \tag{1}$$

The expectation value of x in an arbitrary quantum state $|\Psi(t)\rangle$ can be written as $\langle x\rangle = \langle\Psi(t)|x|\Psi(t)\rangle = \sum_{m,n} C_m{}^* C_n \langle m|x|n\rangle \exp\{i(E_m - E_n)t/\hbar\}$, where E_n and $|n\rangle$ are the energy eigenvalue and the eigenfunction of H and $|\Psi\rangle$ has been expanded in the basis set $|n\rangle$. Now, the perturbation theory comes into play and the energy eigenvalue can be written to $O(\lambda)$) as $E_n = \hbar\omega\{(n + 1/2) + (3\lambda\hbar/8m^2\omega^3)(n^2 + n + 1/2)\}$ while the wave function $\Psi_n(x) = \Psi_{n0}(x) + \lambda\sum_{m\neq n} d_m \Psi_{m0}(x)$, with $d_m = \{\hbar\omega(n - m)\}^{-1} \int \Psi_{m0} * x^4 \Psi_{n0} dx$. To the lowest order in λ, the aperiodic part of $\langle x\rangle$ is that which comes from $\sum_n (C_n C_{n+1} * \exp\{i(E_{n+1} - E_n)\} + C_n C_{n-1}{}^* \exp\{i(E_{n+1} - E_n)/t/\hbar\})$. Since $E_{n+1} - E_n = \hbar\omega\{1 + (3\lambda\hbar/4m^2\omega^3) \times (n + 1)\}$, for arbitrary λ the motion will be quasiperiodic.

What should be noted from the above discussion is the peculiar mixture of nonperturbative and perturbative techniques in showing the quasiperiodicity. The energy difference ΔE_{mn} occurring in the exponential is nonperturbative, while the evaluation of ΔE_{mn} is perturbative. The quantum dynamics should pass over to the classical dynamics if $\hbar \to 0$ or if E_n becomes large, i.e., $n \to \infty$. The latter is apparent from the above discussion, but the former is not. We will show here a way of setting up quantum mechanical perturbation theory which gives the correct classical limit as $\hbar \to 0$.

Our technique will be to construct a quantum mechanical perturbation theory based on the principle of removal of secular terms [1–4]. This is the usual way of doing perturbation theory in classical mechanics where the anharmonic oscillator is handled by an expansion

$$x(t) = x_0(t) + \lambda x_1(t) + O(\lambda^2). \tag{2}$$

In this manner of doing things at $O(\lambda)$, the equation for $x_1(t)$ exhibits resonance which gives rise to secular terms in perturbation theory. The removal of them rests on the realization that the frequency of the perturbed oscillator will be different from its unperturbed frequency ω and there will be an expansion for the frequency in the form [5]

$$\omega* = \omega + \lambda\omega_1 + \lambda^2\omega_2 + . \tag{3}$$

The choice of ω_1 will remove the resonant drive from the equation of x_1. This leads to

$$\omega_1 = (3/8)A^2/m\omega^2. \tag{4}$$

It is well known that secular terms [6] arise in Dirac's time-dependent perturbation theory in quantum mechanics. One of the best known examples is the charged oscillator in a sinusoidal electric field, i.e., the system described by the Hamiltonian ($-e$ is the charge of the oscillator)

$$H = p^2/2m + 1/2m\omega^2 x^2 + eEx\cos\omega t. \tag{5}$$

If the system is known to be in the ground state of the simple harmonic oscillator at $t = 0$, then the probability of its being in the ground state at time t is well known to be

$$\exp(-e^2E^2t^2/8m\hbar\omega) \quad \text{for} \quad t \gg 1/\omega. \tag{6}$$

The second order perturbation theory gives $(1 - e^2E^2t^2/8m\hbar\omega)$ which obviously breaks down for large time because of the t^2 term. This is the effect of the secular term. There have been efforts to remove these sorts of secular terms and they yield ways of forming the perturbation series without indicating the true time dependence given by the exponential term. The perturbation theory that we will describe will not only reproduce the exponential nature of the probability of remaining in the ground state, but will also show that as $\hbar \to 0$

$$\langle X(t)\rangle = x(o)\cos\omega t + [p(0)/m\omega]\sin\omega t - (eE/2m\omega)t\sin\omega t, \quad (7)$$

which is the correct classical solution of the dynamics governed by the Hamiltonian of Eq. (5).

To set up our perturbation theory, we consider a Hamiltonian $H = H_0 + \lambda V(t)$, where we treat $\lambda V(t)$ as the perturbation term and H_0 is the time-independent unperturbed Hamiltonian. Instead of starting with the Schrödinger equation, we start with the equation of motion for the time-evolution operator T. This is where we are drawing the lesson from the initial discussion. We choose to work with an operator that is intrinsically nonperturbative. We recall that $T = \exp(-iHt/\hbar)$ in the time-independent case. The perturbation appears in the exponential by definition. Consequently, although a perturbative technique for calculating T will be set up, the nonperturbative nature will be retained. For later convenience, we work with T^*, which we define as

$$T^* = \exp(iH_0t/\hbar)T, \quad (8)$$

so T^* is the time-evolution operator in the interaction picture. The equation of motion satisfied by T^* is easily seen to be

$$i\hbar dT^*/dt = \lambda V^* T^*, \quad (9)$$

where

$$V^* = \exp(iH_0t/\hbar)V\exp(-iH_0t/\hbar). \quad (10)$$

Now let us try to solve Eq. (9) directly in a perturbative fashion by expanding

$$T^* = T_0{}^* + \lambda T_1{}^* + \lambda^2 T_2{}^* + O(\lambda^3). \quad (11)$$

Clearly,

$$T_0{}^* = \text{ const.} \quad (12)$$

The constant can be chosen to be unity from the initial condition. At the higher orders,

$$i\hbar dT_1{}^*/dt = V^*T_0{}^*, \qquad i\hbar dT_2{}^*/dt = V^*T_1{}^*. \quad (13)$$

If V^* has a time-independent part, $V_0{}^*$, then it is clear from Eq. (13) that $T_1{}^*$ can be written as

$$T_1{}^* = -iV_0{}^*t/\hbar + \text{ other terms}. \quad (14)$$

So, $T_1{}^*$ contains a term that grows linearly with time. This is the secular term and leads to divergence in perturbation theory. Our method will be to treat Eq. (9) in such a manner that secular terms do not appear. To do that we can exploit a technique commonly used in classical nonlinear dynamics called the multiple scale analysis [7]. If we look at Eqs. (12)–(14), we can see that T^* has the structure $1 - i\lambda tV_o{}^*/\hbar +$ other terms. It is when $t \sim 1/\lambda$ that the perturbation theory breaks down. Inspection of Eq. (13) shows that the most secular part of $T_2{}^*$ is quadratic in t and the leading contribution to T^* is $(\lambda t)^2V_0{}^*/2\hbar^2$. It is clear that a shortcut to eliminating the secular terms will be to introduce a new time variable, $\tau = \lambda t$. Even though the exact solution T^* is a function of t and λ, multiple scales analysis seeks solutions which are functions of t, λ, and τ treated as independent variables. We can justify our assertion that T^* may be treated as a function of t, λ, and λt in the following way . We start with the equation of motion of the T^* operator given by Eq. (9).

Now, let $V^*(t)$ contain a time-independent part $V_0{}^*$ and a time-dependent part $\Delta V^*(t)$. So we can write,

$$i\hbar dT^*/dt = [\lambda V_0{}^* + \lambda\Delta V^*(t)]T^*. \quad (15)$$

It is very similar to the equation of motion of the original time-evolution operator T, which is given by

$$i\hbar dT/dt = [H_0 + \lambda V(t)]T, \quad (16)$$

where H_0 is the time-independent unperturbed Hamiltonian. So, by analogy, we can define a second operator T^{**} as

$$T^{**} = \exp(i\lambda V_0{}^*t/\hbar)T^* = \exp(iV_0{}^*\lambda t/\hbar)T^*. \quad (17)$$

T^{**} satisfies the equation of motion

$$i\hbar dT^{**}/dt = \lambda V^{**}(t)T^{**}, \quad (18)$$

where

$$V^{**}(t) = \exp(iV_0{}^*\lambda t/\hbar)\Delta V^*(t)\exp(-iV_0{}^*\lambda t/\hbar). \quad (19)$$

We can repeat the above procedure *as long as the transformed potentials contain time-independent parts.* It is clear from the form of the transformed potential, $V^{**}(t)$, that the time-independent part which comes out of it will be at least of the first order in λ. As a result, the transformed operator T^{***} will have a form very similar to T^{**} except that λt will be replaced by $\lambda^2 t$ and T^* by T^{**}. If we assume that the process stops after n steps, then the nth transformed operator can be written in the form

$$T^{(n)} = f(\lambda t, \lambda^2 t, \lambda^3 t, \ldots \lambda^n t)T^*$$

or

$$T^* = f^{-1}T^{(n)}.$$

That f is invertible is evident from its exponential structure. We can see that T^* may be considered as a function of λ, t, and λt and they can be treated as independent. The dependence on other variables can be ignored as they depend on higher powers of λ. So, T^* exhibits multiple-time scale behavior and it is a strictly nonperturbative result.

We emphasize that writing T^* as a function of two time variables is an artifice to remove secular terms; the actual solution has t and τ related by $\tau = \lambda t$, so that t and τ are not ultimately independent.

We can formally expand T^* as

$$T^* = {T_0}^*(t,\tau) + \lambda {T_1}^*(t,\tau) + \lambda^2 {T_2}^*(t,\tau) + O(\lambda^3) \quad (20)$$

and the time derivative as

$$dT^*/dt = \partial {T_0}^*/\partial t + \lambda \partial {T_0}^*/\partial\tau + \lambda \partial {T_1}^*/dt + \lambda^2 \partial {T_1}^*/\partial\tau + \ldots.. \quad (21)$$

Inserting the above expansion in Eq. (9) and equating term by term, we have

$$i\hbar \partial {T_0}^*/\partial t = 0, \quad (22)$$

$$i\hbar(\partial {T_0}^*/\partial\tau + \partial {T_1}^*/\partial t) = V^* {T_0}^*, \quad (23)$$

$$i\hbar(\partial {T_1}^*/\partial\tau + \partial {T_2}^*/\partial t) = V^* {T_1}^*, \quad (24)$$

and so on.

From Eq. (22), it is clear that ${T_0}^*$ is a function of τ alone. We are free to choose this according to our convenience. We now write V^* as ${V_0}^* + \Delta V^*(t)$, where ${V_0}^*$ is the time-independent part of V^* and $\Delta V^*(t) = V^* - {V_0}^*$ and choose ${T_0}^*$ as

$$i\hbar \partial {T_0}^*/\partial\tau = {V_0}^* {T_0}^*. \quad (25)$$

The time dependence of ${T_1}^*$ is now given by (see Eq. (23))

$$i\hbar \partial {T_1}^*/\partial t = \Delta V^*(t) {T_0}^*. \quad (26)$$

The solution of this equation can be written as

$${T_1}^* = (-i/\hbar)\left[\int^t \Delta V^*(t')dt'\right]{T_0}^* + f(\tau), \quad (27)$$

where the lower limit of integration is 0 and $f(\tau)$ is a function of τ only, whose form will be chosen to remove the secular term from ${T_2}^*$ as shown below. The equation of motion of the ${T_2}^*$ is found to be

$$i\hbar \partial {T_2}^*/\partial t = \Delta V^*(t)\left\{(-i/\hbar)\int^t \Delta V^*(t')dt'\right\}{T_0}^* + \left[{V_0}^*, (-i/\hbar)\int^t \Delta V^*(t')dt'\right]{T_0}^* - i\hbar df/d\tau + V^*(t) f(\tau). \quad (28)$$

Now we choose $f(\tau)$ to remove the t-independent part from the right-hand side of Eq. (28). This leads to the equation

$$-i\hbar df/d\tau + {V_0}^* f(\tau) + c{T_0}^*(\tau) = 0, \quad (29)$$

where ${V_0}^*$ is the constant part of $V^*(t)$ and c is the t-independent part associated with ${T_0}^*(\tau)$. Equation (29) together with the boundary condition $f(0) = 0$ uniquely determines $f(\tau)$. The same process has to be repeated at every stage to get the full perturbation series. So ${T_0}^*$ can be written as

$$T^* = \exp(-i{V_0}^*\tau/\hbar) + \lambda\{(-i/\hbar)\left[\int^t \Delta V^*(t')dt'\right]{T_0}^* + (-i/\hbar){T_0}^* \int^\tau {T_0}^{*-1} c {T_0}^* d\tau\} + O(\lambda^2). \quad (30)$$

This is the principal result and hence it is worth understanding the content in a different fashion. We return to Eq. (13) and note that the nth order T^* satisfies $i\hbar d{T_n}^*/dt = V^* {T_{n-1}}^*$. To obtain the leading order secular term, we note that the time-independent part ${V_0}^*$ of V^* is necessary and if ${T_{n-1}}^* = {V_0}^{*n-1} t^{n-1}/(n-1)!1/(i\hbar)^{n-1}$ then ${T_n}^* = {V_0}^{*n} t^n/n!(i\hbar)^n$ leading to $T^* = 1 + \sum_n \lambda^n {V_0}^{*n} t^n/n!(i\hbar)^n = \exp(-i{V_0}^*\lambda t/\hbar)$. This is exactly the zeroth order answer obtained in Eq. (13), which thus represents the sum of the most secular term at every order of perturbation theory.

In the remainder of the Letter, we demonstrate the efficacy of the zeroth order answer for T^*. We begin with the charged oscillator with the Hamiltonian given by Eq. (5). The quantity V^* in this case is given by

$$V^* = 1/2\exp(iH_0 t/\hbar)x[\exp(i\omega t) + \exp(-i\omega t)] \times \exp(-iH_0 t/\hbar). \quad (31)$$

Writing x in terms of the creation and annihilation operators a^+ and a of H_0 and recognizing that $\exp(iH_0 t/\hbar) a \exp(-iH_0 t/\hbar) = a(0)\exp(-i\omega t)$, we find the time-independent part of V^* to be given by

$${V_0}^* = 1/2X(0). \quad (32)$$

From Eq. (30),

$$T^* = \exp(-i{V_0}^*\tau/\hbar) + O(\lambda) \Rightarrow T = \exp(-iH_0 t/\hbar)\exp(-ieExt/2\hbar) + O(\lambda).$$

Surprisingly enough, the above equation reproduces correctly the probability of the system remaining in the ground state at time t (for $t \gg 1/\omega$) if it were in the ground state at $t = 0$. This probability $P(t)$ is

$$P(t) = |\langle 0|\Psi(t)\rangle|^2 = |\langle 0|T|0\rangle|^2. \quad (33)$$

The probability can be easily calculated and is given by Eq. (6).

The operator $X(t)$ in the Heisenberg picture is found from

$$X(t) = T^{-1}X(0)T = X(0)\cos\omega t + \exp(ieExt/2\hbar)(P(0)/m\omega) \times \sin\omega t \exp(-ieExt/2\hbar).$$

The second term on the right-hand side can be evaluated by the Baker- Campbell-Hausdorff theorem to obtain

$$X(t) = X(0)\cos\omega t + (P(0)/m\omega)\sin\omega t - eEt\sin\omega t/2m\omega. \quad (34)$$

Taking expectation value reduces this operator expression to the usual classical result.

We next discuss the anharmonic oscillator given by Eq. (1). The quantity V^* is $1/4\exp(iH_0t/\hbar)x^4\exp(-iH_0t/\hbar)$ and to evaluate $V_0{}^*$, the time-independent part of V^*, we write x in terms of the creation and the annihilation operators of H_0 to write

$$x^4/4 = (\hbar^2/16m^2\omega^2)(a - a^+)^4. \tag{35}$$

The number operator $N = a^+a$ commutes with H_0 and hence the part of Eq. (35) which is expressible in terms of N and the unit operator are the contributions to $V_0{}^*$. Straightforward algebra yields

$$V_0{}^* = (3\hbar^2/16m^2\omega^2)(2N^2 + 2N + 1). \tag{36}$$

Steps similar to those carried out before lead to

$$\begin{aligned} X(t) = {} & \exp\{(3/8)(i\lambda\hbar t/m^2\omega^2)(N^2 + N + 1/2)\} \\ & \times\{X(0)\cos\omega t + [P(0)/m\omega]\sin\omega t\} \\ & \times\exp\{-(3/8)(i\lambda\hbar t/m^2\omega^2)(N^2 + N + 1/2)\}. \end{aligned} \tag{37}$$

We now expand the right-hand side of Eq. (37) to $O(\lambda)$ and take the limit of $\hbar \to 0$ and compare with the corresponding classical result. We find that

$$\begin{aligned} X(t) = {} & X(0)\cos\omega t + (P(0)/m\omega)\sin\omega t + (3/8) \\ & \times (i\lambda\hbar t/m^2\omega^2)) \times [N^2 + N + 1/2, X(0)\cos\omega t \\ & + (P(0)/m\omega)\sin\omega t]. \end{aligned} \tag{38}$$

Noting that $N = H_0/\hbar\omega - 1/2$, it is clear that as $\hbar \to 0$, terms like $[N, X(0)]$ or $[N, P(0)]$ do not contribute and further that only $[N^2, X(0)]$ and $[N^2, P, (0)]$ survive in the limit of $\hbar \to 0$. In that limit to $O(\lambda)$

$$\begin{aligned} X(t) = {} & X(0)\{\cos\omega t - (3/8)(\lambda/m\omega)X^2(0)t\sin\omega t\} \\ & + \text{ other terms in } (P(0)). \end{aligned} \tag{39}$$

The expectation value of the above equation when taken with the choice $\langle P(0)\rangle = 0$ leads to the classical limit

$$X_{\rm cl}(t) = A[\cos\omega t - (3/8)(\lambda/m\omega)A^2t\sin\omega t], \tag{40}$$

which is to be compared with answer according to Eqs. (3) and (4)

$$\begin{aligned} X(t) &= A\cos\omega^* t = A\cos\{\omega + (3/8)(\lambda A^2 m\omega^2)\}t \\ &= A[\cos\omega t - (3/8)(\lambda A^2/m\omega^2)t\sin\omega t + O(\lambda)]. \end{aligned} \tag{41}$$

We have also checked that Eq. (37) exactly reproduces the classical Eq. (41) in the limit $\hbar \to 0$ (taking the limit $\hbar \to 0$ is equivalent to treating the quantum operators in Heisenberg picture as classical dynamical variables).

Thus, our perturbation theory reproduces the correct classical result as $\hbar \to 0$. In conclusion, we would like to reiterate that the multiple scale perturbation theory can be exploited to set up a general time-dependent perturbation theory in quantum mechanics and this perturbation theory has a smooth classical limit.

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