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On the time-dependent perturbation theory

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Abstract. It is shown that if the time-dependent perturbation Hamiltonian admits of Fourier resolution, then the solution of the wave equation possesses perturbation expansions, without any secular term. Further, each term can be expressed in terms of its Fourier resolution.

1. Introduction

The object of this short paper is to develop a perturbation expansion for the wave function of a system acted on by a time-dependent perturbation where the Hamiltonian due to the perturbation may be expressed in Fourier integral form. Even for systems with a periodic or oscillatory perturbation, one encounters serious difficulty due to the presence of so-called secular terms, i.e. terms of the type $P(t)T(t)$, where $P(t)$ is a polynomial and $T(t)$ is a trigonometric function of time t. These unphysical terms appeared in the study of classical celestial mechanics in the last century and Poincaré (1895) developed methods to obtain oscillatory solutions for such systems. More recently Krylov and Bogoliubov (1937) and later Bogoliubov and Mitropolsky (1958) have developed perturbation methods to obtain asymptotic solutions without secular terms. These methods are undoubtedly very powerful in the sense that they are applicable to quite general time-dependent problems and further, they are extremely useful in nonlinear problems.

In quantum mechanics, the equations are linear, which simplifies the situation enormously. During the last forty years there have been quite important developments in the general theory of linear differential equations and in particular of those with periodic coefficients. In developing a time-dependent perturbation theory it seems to be more apt to utilize these results. Let

$$\frac{\mathrm{d}X}{\mathrm{d}t} = \Pi(t)X \tag{1}$$

where X is the unknown vector and $\Pi(t)$ is a periodic matrix such that

$$\Pi(t+\tau) = \Pi(t).$$

It is well known (Halany 1963) that the solution which is X_0 at t_0 is of the form

$$X(t) = \Gamma(t)\exp\{\Omega(t-t_0)\}\Gamma^{-1}(t_0)\,X_0 \tag{2}$$

where the matrix $\Gamma(t)$ is periodic such that $\Gamma(t+\tau) = \Gamma(t)$. This is a generalization of Floquet's theorem for a single unknown function (Ince 1926). The constant matrix Ω known as monodormy matrix, can be shown to be diagonalizable so that instead of working with any arbitrary X_0, if $\Gamma^{-1}(t_0)\,X_0$ is an eigenvector Y of eigenvalue μ of Ω then

$$X(t) = \exp\{\mu(t-t_0)\}\Gamma(t)\,Y. \tag{3}$$

Hence, in an adequate perturbation theory both the index μ and the vector $\Gamma(t)Y$ should be expanded in ascending powers of the perturbation parameter ϵ so that the Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \{H_0+\epsilon H_1(t)\}\Psi \tag{4}$$

where H_0 is the unperturbed Hamiltonian which does not depend on time, should have solution of the form

$$\Psi = \exp\left\{-\frac{i}{\hbar}(\epsilon\lambda^{(1)}+\epsilon^2\lambda^{(2)}+\ \dots)t\right\}\sum_k \exp\left\{-\frac{i}{\hbar}E_j t\right\}\varphi_k$$
$$\times\ (a_k^{(0)}+\epsilon a_k^{(1)}+\epsilon^2 a_k^{(2)}+\ \dots). \tag{5}$$

$H_1(t+\tau) = H_1(t)$ and ϵ is the perturbation parameter. φ_k are eigenfuctions of H_0 with eigenvalues E_k. $a_k^{(N)}(t)$ are periodic, i.e. $a_k^{(N)}(t+\tau) = a_k^{(N)}(t)$. It may be recalled that in the theory of nonlinear oscillations one also starts from expansions which are to some extent similar to the expression (5), Krylov–Bogoliubov (1937).

When $H_1(t)$ is not periodic but has the Fourier resolution

$$H_1(t) = \int_{-\infty}^{\infty} H(\omega)\exp(i\omega t)\,d\omega \tag{6}$$

the form of the expansion (5) suggests that one should attempt a perturbation expansion of the solutions, equation (4) in the form

$$\Psi = \exp\left\{-\frac{i}{\hbar}(\epsilon\lambda^{(1)}+\epsilon^2\lambda^{(2)}+\ \dots)t\right\}\sum_k \exp\left(-\frac{i}{\hbar}E_k t\right)\varphi_k$$
$$\times\ \{A_k^{(0)}+\epsilon A_k^{(1)}(t)+\epsilon^2 A_k^{(2)}(t)+\ \dots\} \tag{7}$$

where $\lambda^{(N)}$ are constant and $A_k^{(N)}(t)$ have the Fourier resolution

$$A_k^{(N)}(t) = \int_{-\infty}^{\infty} A_k^{(N)}(\omega)\exp(i\omega t)\,d\omega. \tag{8}$$

This suggestion is *a posteriori* justified in § 2 in the case of separable Hilbert space. Thus we arrive at solutions which no longer contain secular terms.

The nature of the solutions thus obtained is studied in § 3; it is shown that they form a complete orthonormal set. The initial-value problem is investigated in § 4, where the solution evolving from any arbitrary initial state is obtained. § 5 is devoted to the solution of the secular equation so as to obtain the characteristic unperturbed states, which are linear combinations of the unperturbed solutions. In § 6 we have studied the special cases (i) the periodic perturbation and (ii) the perturbation is the sum of two individually periodic terms with different periods. The last section is a general discussion on the method.

2. The perturbation expansion

We assume that the eigenvalues E_k of H_0, are discrete and the eigenfunctions φ_k form a complete orthonormal set; further, they are known already. It is clear from equation (7) that the starting unperturbed solution is to be taken as a linear combination of steady-state solutions of H_0, i.e.

$$\Psi^{(0)} = \sum_k A_k^{(0)} \exp\left(-\frac{\mathrm{i}}{\hbar} E_k t\right)\varphi_k, \qquad \sum_k |A_k^{(0)}|^2 = 1. \tag{9}$$

The constants $A_k^{(0)}$ are as yet arbitrary but for the above restriction due to normalization. Substituting the expression (6) for H_1 in equation (4) and equating the coefficients of ϵ^N on both sides, we get for $N \geqslant 1$

$$\mathrm{i}\hbar \frac{\mathrm{d}A_k^{(N)}}{\mathrm{d}t} = \sum_l \int_{-\infty}^{\infty} \{H_{kl}(\omega)\, \mathrm{e}_{kl}(\omega) - \lambda^{(1)}\delta_{kl}\} A_l^{(N-1)} \mathrm{d}\omega - \sum_{M=1}^{N-2} \lambda^{(N-M)} A_k^{(M)}. \tag{10}$$

In the above we have used the abbreviation

$$H_{kl}(\omega) = (\tilde{\varphi}_k H(\omega)\varphi_l) \quad \text{and} \quad \mathrm{e}_{kj}(\omega) = \exp\left\{\frac{\mathrm{i}}{\hbar}(E_k - E_j + \hbar\omega)t\right\}. \tag{11}$$

These equations can be integrated successively starting from $N = 1$. The constants $\lambda^{(N)}$ are to be determined such that the $A_k^{(N)}(t)$ have Fourier resolutions as given in equation (8). Thus for, $N = 1$,

$$\mathrm{i}\hbar \frac{\mathrm{d}A_k^{(1)}}{\mathrm{d}t} = \sum_l \left[\int_{-\infty}^{\infty} \left\{H_{kl}(\omega) - H_{kl}\left(\frac{E_l - E_k}{\hbar}\right)\right\} \mathrm{e}_{kl}(\omega)\, \mathrm{d}\omega + \left\{2\pi H_{kl}\left(\frac{E_l - E_k}{\hbar}\right) - \lambda^{(1)}\delta_{kl}\right\} A_l^{(0)}\right]. \tag{12}$$

The integrand on the right-hand side is so written that it is zero at $\omega = (E_l - E_k)/\hbar$; thus the integral exists if $H_{kl}(\omega)$ is differentiable at $\omega = (E_l - E_k)/\hbar$. We will assume it to be so; hence, the integration can be carried out in a straightforward manner.

2.1. *The unperturbed solution*

Thus $A_k^{(1)}(t)$ will not have any secular term and will be of the form (8) if we choose $\lambda^{(1)}$ and $A_k^{(0)}$ such that

$$\sum_l \left\{H_{kl}\left(\frac{E_l - E_k}{\hbar}\right) - \frac{\lambda^{(1)}}{2\pi}\delta_{kl}\right\} A_l^{(0)} = 0. \tag{13}$$

This is an eigenvalue problem. The order of this secular determinant is that of the dimension of the space of unperturbed eigenfunctions. Though the problem becomes more and more complicated with the increase of dimension, it is not unwieldy and one can solve the problem by successive approximation if one notes the restriction on $H_{kl}\{(E_l - E_k)/\hbar\}$ due to the physical nature of the problem and the convergence of the integral (8). We will take up this in § 5.

We observe, here, that from the hermiticity of H_1 it follows

$$H_{kl}\left(\frac{E_l - E_k}{\hbar}\right) = H_{lk}^*\left(\frac{E_k - E_l}{\hbar}\right).$$

Hence, the eigenvalues $\lambda_\alpha^{(1)}$ are real and the eigenvectors A_α are orthonormal. The equations (13) and (9) show that if we want the solution to have the stipulated property we cannot start with any arbitrary unperturbed solution but those linear combinations formed by the eigenvector of $H_{jk}\{(E_k - E_j)/\hbar\}$. In order to specify this starting unperturbed solution we use the subscript α to denote the solution Ψ_α which corresponds to the eigenvalues $\lambda_\alpha^{(1)}$ and the eigenvectors A_α of equation (13), such that

$$\Psi_\alpha \to \sum A_{\alpha k} \exp\left(-\frac{\mathrm{i}}{\hbar} E_k t\right) \varphi_k \quad \text{as } \epsilon \to 0. \tag{5'}$$

2.2. *First-order terms*

It follows from equation (11) that

$$A_{\alpha k}^{(1)} = -\sum_l \int_{-\infty}^{\infty} \bar{H}_{kl}(\omega)\, \mathrm{e}_{kl}(\omega)\, \mathrm{d}\omega A_{\alpha l} + \mathrm{i} \sum_\beta b_{\alpha\beta} A_{\beta k} \tag{14}$$

where we have used the notation

$$\bar{F}_{kl}(\omega) = \frac{F_{kl}(\omega) - F_{kl}\{(E_l - E_k)/\hbar\}}{E_k - E_l + \hbar\omega}. \tag{14'}$$

In order that the Ψ_α are orthonormal the matrices $\{b_{\alpha\beta}\}$ which are constants, should be Hermitian, they are to be determined from second-order terms. One may recall the similarity of this procedure, of choosing the linear combination of unperturbed states and determining the constants of integration from next higher-order terms, to that followed in the degenerate time-independent perturbation theory (Born *et al.* 1926). It is also similar to that in the case of the Krylov–Bogoliubov theory of non-linear oscillations.

2.3. *Second-order terms*

We substitute the expression (14) for $A_{\alpha k}^{(1)}$ in equation (10) for $N = 2$ and proceed exactly in the same manner as in the previous case to choose $\lambda_\alpha^{(2)}$ and b so that the right-hand side can be integrated in a straightforward way. Thus

$$\lambda_\alpha^{(2)} A_{\alpha k} + \mathrm{i} \sum_\beta (\lambda_\alpha^{(1)} - \lambda_\beta^{(1)}) b_{\alpha\beta} A_{\beta k} = \sum_j B_{kj}\left(\frac{E_j - E_k}{\hbar}\right) A_{\alpha j} \tag{15}$$

where

$$B_{kj}(x) = \sum_l \int_{-\infty}^{\infty} H_{kl}(x-y) \bar{H}_{lj}(y)\, \mathrm{d}y. \tag{15'}$$

Hence

$$\left.\begin{aligned} \lambda_\alpha^{(2)} &= \sum_{k,j} A_{\alpha j} A_{\alpha k}^* B_{kj}\left(\frac{E_j - E_k}{\hbar}\right) \\ \text{and} \qquad b_{\alpha\beta} &= \frac{\mathrm{i}}{\lambda_\beta^{(1)} - \lambda_\alpha^{(1)}} \sum_{k,j} B_{kj}\left(\frac{E_j - E_k}{\hbar}\right) A_{\alpha j} A_{\beta k}^*. \end{aligned}\right\} \tag{16}$$

Finally

$$\begin{aligned} A_{\alpha k}^{(2)} = \mathrm{i} \sum_\beta f_{\alpha\beta} A_{\beta k} &+ \sum_j \int_{-\infty}^{\infty} \bar{B}_{kj}(\omega)\, \mathrm{e}_{kj}(\omega)\, \mathrm{d}\omega A_{\alpha j} \\ &- \sum_l \int_{-\infty}^{\infty} \{\mathrm{i}\bar{H}_{kl}(\omega) \sum_\beta b_{\alpha\beta} A_{\beta l} + \lambda_\alpha^{(1)} \bar{\bar{H}}_{kl}(\omega) A_{\alpha l}\}\, \mathrm{d}\omega\, \mathrm{e}_{kl}(\omega) \end{aligned} \tag{17}$$

where the $f_{\alpha\beta}$ are constants. We can proceed in this way to any higher-order terms. The question of convergence of the series will not be taken up here.

3. The characteristic solutions

The solutions obtained above may be made orthonormal. This is evident from equation (4), as $\{\tilde{\Psi}_\alpha(t)\Psi_\beta(t)\}$ is constant and one can choose the constant to be independent of ϵ. So that

$$\{\tilde{\Psi}_\alpha(t)\Psi_\beta(t)\} = \{\tilde{\Psi}_\alpha^{(0)}(t)\Psi_\beta^{(0)}(t)\} = \delta_{\alpha\beta}. \tag{18}$$

Next, it is clear from above that to each $\Psi_\alpha^{(0)}(t)$ there corresponds a $\Psi_\alpha(t)$ and $\Psi_\alpha^{(0)}(t)$ is obtained from φ_k by a unitary transformation. Hence, the solutions $\Psi_\alpha(t)$ form a complete set. Thus one can write

$$\Psi_\alpha(t) = \sum_k U_{\alpha k}(t)\varphi_k \tag{19}$$

where $\{U_{\alpha k}\}$ is unitary, the elements of which are given by equations (7), (8), (14) and (17). The characteristic solutions are the interesting ones from the physical point of view and their role is the same as that of steady states in the unperturbed system.

4. The initial-value problem

It follows that the most general solution of equation (4) is a linear combination of the $\Psi_\alpha(t)$. So that one can easily find the solution which evolves out of any arbitrary initial state, either a pure or a mixed one. Let the initial state at $t = t_0$ be $\Psi(t_0)$, since the φ_k form a complete set, $\Psi(t_0)$ can be expressed as

$$\Psi(t_0) = \sum_k \{\tilde{\varphi}_k\Psi(t_0)\}\varphi_k. \tag{20}$$

It is easy to verify that $\Psi(t)$ which at $t = t_0$ is $\Psi(t_0)$ may be expressed as a linear combination of $\Psi_\alpha(t)$ as

$$\Psi(t) = \sum_\alpha g_\alpha\Psi_\alpha(t) \tag{21}$$

where

$$g_\alpha = \sum_k U_{\alpha k}^*(t_0)\{\tilde{\varphi}_k\Psi(t_0)\}. \tag{22}$$

5. The characteristic unperturbed states

Our investigation shows that if the time-dependent perturbing operator possesses Fourier resolution, a perturbation expansion of the wave function can be found where each term admits of Fourier resolution. One can simply write down the expansion in terms of the eigenvalues and eigenvectors of the secular equation (13). In general it is not possible to write the solutions of this equation in a closed form. However, the existence of the integral (6) demands that $|H_{kj}(\omega)| \to 0$ very rapidly with $|\omega| \to \infty$. Further, in most of the physical problems the spectra are concentrated in small frequency intervals, hence the effective contribution is only from a small number of terms. The nature of these unperturbed states is characteristic of the perturbation and there cannot be a general rule to write them down. Here we will discuss two special cases to obtain them.

5.1. *The low-frequency spectrum*

The spectra are concentrated in the low-frequency region. In this case, the effective contributions are only from H_{jj}, $H_{j(j+1)}$. Neglecting higher powers of small ratios,

$\lambda_n^{(1)}$ and A_{nm} are given by

$$\left.\begin{aligned} \lambda_n^{(1)} &= H_{nn} + \frac{|H_{n(n+1)}|^2}{H_{(n+1)(n+1)} - H_{nn}} + \frac{|H_{n(n-1)}|^2}{H_{(n-1)(n-1)} - H_{nn}} \\ A_{nn} &= 1, \qquad A_{n(n\pm 1)} = kH_{n(n\pm 1)} \\ H_{(n\pm 1)(n\pm 2)}A_{n(n\pm 2)} &= k(H_{nn} - H_{(n\pm 1)(n\pm 1)})H_{n(n\mp 1)} - H_{(n\pm 1)n}. \end{aligned}\right\} \tag{23}$$

If there is degeneracy, one has to start with suitable linear combinations, such that in this subspace it diagonalizes H_{jk}. The arguments of H_{nm} are $(E_n - E_m)/\hbar$. k is a constant.

5.2. *Resonant case*

In the case of resonance, i.e. the spectra are mostly concentrated at $(E_1 - E_2)/\hbar$ (say); so that $|H_{12}|$ is very large and $H_{n(n\pm 1)}$ are the only remaining effective terms. Neglecting higher order of small ratios,

$$\left.\begin{aligned} \lambda_\pm^{(1)} &= \pm\Big(\sum_n |H_{n(n+1)}|^2\Big)^{1/2}, \qquad \lambda_n^{(1)} \simeq 0 \quad \text{for } n \geqslant 3 \\ (\lambda_\pm^2 + |H_{12}|^2)^{1/2}A_\pm &= (H_{12}, -\lambda_\pm, 0, 0, \dots), \qquad A_{nk} \simeq \delta_{nk} \quad \text{for } n \geqslant 3. \end{aligned}\right\} \tag{24}$$

Here, two of the characteristic unperturbed states are linear combinations of φ_1 and φ_2. As a matter of fact if $H'(t) = \epsilon H^0 \cos(\omega t + \delta)$ the above solutions (equation (24)) are exact.

6. Special cases

In this section we wish to study the nature of the solutions in some particular cases which are important from a physical standpoint.

(i) The time-dependent perturbation is periodic which encompasses a large number of problems. So that

$$H(\omega) = \sum_{-\infty}^{\infty} H(n)\delta(\omega - n\omega_0). \tag{25}$$

In the case $E_k - E_l \neq n\omega_0$, it is readily observed that $H_{kl}\{(E_l - E_k)/\hbar\}$ is diagonalized in the space of unperturbed eigenvectors φ_k, hence, they are the characteristic unperturbed states and $\Psi_k(t) \to \varphi_k \exp\{-(\mathrm{i}/\hbar)E_k t\}$ as $\epsilon \to 0$. The solutions retaining first-order terms are given by

$$\Psi_k^1 = \exp\left\{-\frac{\mathrm{i}}{\hbar}\epsilon H_{kk}^{(0)}t\right\} \sum_{-\infty}^{\infty} \sum_j \exp\left(-\frac{\mathrm{i}}{\hbar}E_k t\right)\varphi_j H_{jk}(n) \times \left(\frac{1 - \delta_{jk}\delta_{n0}}{E_k - E_j - n\hbar\omega_0}\right)\exp(\mathrm{i}n\omega_0 t). \tag{26}$$

It may be possible to absorb the diagonal elements $H_{kk}^{(0)}$ in the unperturbed Hamiltonian, to get rid of the first exponential factor, but this cannot be continued in the second-order where the coefficient $\lambda_k^{(2)}$ in expression (5) is

$$\lambda_k^{(2)} = \sum_{-\infty}^{\infty} \sum_l \left\{\frac{H_{kl}(m)H_{lk}(-m)(1 - \delta_{m0})}{E_k - E_l + m\hbar\omega_0} + \frac{|H_{kk}^{(0)}|^2(1 - \delta_{kl})}{E_k - E_l}\right\}. \tag{27}$$

In general $\lambda_k^{(2)} \neq 0$ and they manifest some interesting effects of second-order terms, e.g. the intensity-dependent frequency shift in scattering problems (Kibble 1964, Eberly and Reiss 1966, Goldman 1964, Sen Gupta 1967).

(ii) Next, let us consider

$$H_1 = \sum_{-\infty}^{\infty} \{H'(n)\,\delta(\omega - n\omega_1) + H''(n)\,\delta(\omega - n\omega_2)\} \tag{28}$$

i.e. the perturbation consists of two periodic terms. A special case of which is the problem of electrons in the field of two electromagnetic beams; this has been studied by Reiss (1962) and the author (Sen Gupta 1966). We will restrict our discussion to the case $E_k - E_l \neq n\omega_i h$ for $i = 1, 2$. In this case also H_0 is already diagonal and the expression for $\lambda_k^{(1)}$ and $A_k^{(1)}$ similar to those in (26) may be obtained. However, in second- and higher-order terms, a physically interesting situation appears owing to the possibility of absorption of $\hbar\omega_1$, and emission of $\hbar\omega_2$ and vice-versa. However, the expressions at this stage become highly involved so that they should be better taken up separately. These transitions are enhanced when $E_k - E_l = \hbar(n\omega_1 - m\omega_2)$.

7. Discussion

Let us examine the nature of the solutions we have found and let us compare them with the solutions which are obtained from the conventional time-dependent perturbation theory. The first point to be noted is the first exponential factor in the expression (7), the index of which is a power series in ϵ, the perturbation parameter. It is clear that if one expands the solution directly in powers of ϵ, as it is done in the usual time-dependent perturbation theory, then each term increases indefinitely with t. This is one of the reasons for the appearance of secular terms in the usual perturbation theories. The other important point is that the characteristic unperturbed solutions are not, in general, eigenfunctions of the unperturbed Hamiltonian (even in the first-order of small quantities)—as is clear from § 5.2 in the case of resonance. This is tacitly assumed in the usual time-dependent perturbation theory. Thus it is possible to obtain solutions without secular terms even in case of resonance. They are of physical interest as they manifest the second- and higher-order effects. With the advent of very high-intensity fields their contributions may no longer be negligible. We intend to investigate the transition rates in general and in the presence of resonance in future. Finally, the method followed here may be extended, though only in some special cases, to systems in which the eigenvalues are no longer discrete.

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