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Autor(en): **Martin, Ph.A. / Nenciu, G.**

Objekttyp: **Article**

Zeitschrift: **Helvetica Physica Acta**

Band (Jahr): **65 (1992)**

Heft 4

PDF erstellt am: **25.04.2024**

Persistenter Link: https://doi.org/10.5169/seals-116503

Helv Phys Acta
Vol. 65 (1992)

0018-0238/92/040528-32$1.50+0.20/0

Perturbation theory for time dependent hamiltonians : rigorous reduction theory

Ph. A. Martin
Institut de Physique Théorique, EPFL
PHB-Ecublens - CH-1015 Lausanne, Switzerland

and

G. Nenciu
Department of Theoretical Physics
University of Bucharest, Bucharest, Romania

(15. VII. 1991, revised 15.XII. 1991)

Abstract

We generalize the standard time independent perturbation theory by constructing time dependent families of orthogonal projections associated with isolated parts σ_0 of the spectrum of the unperturbed hamiltonian. The full evolution between times t_0 and t intertwines approximately these projections up to an error of order $\lambda^{N+1} | t-t_0 |$, where λ is the coupling constant and N + 1 is the lowest order at which σ_0 becomes resonant with the rest of the spectrum. This provides a rigorous basis for deriving effective hamiltonians for time dependent perturbations.

I. INTRODUCTION

For a long time the Dirac's variation of constant method has provided the basis for perturbative solutions of the time dependent Schrödinger equation

$$i\frac{d}{dt}U(t, t_o) = \left(H_o + \lambda V(t)\right) U(t, t_o), \qquad U(t_o, t_o) = I \tag{1.1}$$

The most common examples of (1.1) are atoms or molecules subjected to external electromagnetic fields or spin systems in time variable magnetic fields. When, with the advent of intense laser fields, it was necessary to push the perturbation theory to orders higher than the first non vanishing one the method has been confronted with the problem of so called "secular divergences". It has been early realised that some of these divergences (i.e. terms containing factors of the form λt) are spurious in the sense that they origin in the expansion of an overall phase which does not affect the physical measurable quantities. So the natural idea was first to factorise out the phase factor and only after that to perform the perturbative expansion. For the case when one starts with a non-degenerate eigenvector of H_o and the Fourier transform of $V(t)$ vanishes outside a small neighborhood of the origin (i.e. there are no resonant transitions in the low orders of the perturbation expansion) a factorisation procedure has been (at a formal level) worked out in [1] (this paper contains a thorough discussion of the early developments). Our results below can be viewed as the extension at a rigorous level and by a different method of the factorisation in [1] for the cases when the perturbation couples resonantly some of the eigenstates of H_o. Of course what is factored out is an unitary evolution in the "resonant" subspace.

One way to cope with the perturbation theory for (1.1) is to translate it in the time independent formalism using the Howland method [2]. Unfortunately, the time independent perturbation problem that one obtains in this way is in general also a complicated one. However, there is a particular case for which this method works nicely : the one frequency case i.e.

$$V(t) = V \cos \omega t \tag{1.2}$$

In this case the Howland scheme coincides basically with the so called Floquet (quasi-energy) formalism which has been much used in the atomic physics [3, 4] and references therein]. In particular, combining the Floquet theory with dilation

analiticity (complex scaling) [5, 6] it was possible to develop a fairly detailed rigorous theory of the a.c. Stark effect in atoms (see e.g. [7-11] and references therein). Let us note, however, that the techniques are quite elaborated and not easy to extend; the existence of the Rabi oscillations have been rigorously proved only for the two-body case [10]. Our aim is to obtain (somewhat less detailled) results in less stringent conditions (e.g. for non rectangular laser pulses [12] which amounts to relax the one frequency requirement).

The starting point is the well known fact of the existence of different time scales in the problem : different processes become significant at different time scales and consequently have to be treated by different means; for example in the case of the one or two-photon Rabi oscillations (see e.g. [13]) the radiative damping (ionisation probability) is weak at the appropriate time scale and should be treated perturbatively while the resonant transitions leading to the Rabi oscillations are to be treated nonperturbatively. One can try first to neglect completely the non-resonant transitions and to solve the problem in the "resonant subspace" (the bare N level atom problem) and then to add the influence of the non-resonant transition by perturbation theory, but this approach is not free of difficulties. The alternative is to "decouple" first by perturbation theory the evolution in the resonant subspace from that involving the remainder of the Hilbert space, i.e. to block-diagonalise (up to some order) the time evolution and then solve nonperturbatively the dynamics within the decoupled resonant subspace (the "dressed" N level atom problem). The corresponding hamiltonian in the resonant subspace is usually called "effective hamiltonian". Note that this is the analog of the well known "reduction scheme" of the time independent perturbation theory [14].

A remark is in order here. In the case of nonsingular time independent perturbations, beside the Kato-Rellich analytic perturbation theory [14, 15], there exist alternative methods for deriving effective hamiltonians; the most popular are the Feschbach projection method and the method of canonical transformations (see e.g. [16], [3]). Moreover, at the heuristic level, the projection method has been extended to the "resonant" case (leading to a nonselfadjoint effective hamiltonian) as well as to the time dependent perturbations [16], [3]. It would be interesting to put these formal manipulations on a firm mathematical basis. Let us mention finally that since the effective hamiltonians are unique only up to a unitary

transformation in the "resonant" subspace, care must be taken when comparing the effective hamiltonians given by various methods.

The problems to be solved in this approach are as follows :

i) Develop a perturbation scheme for the (approximate) block diagonalisation of the evolution; since in general the perturbation theory may not converge one has to stop at some finite order and to obtain estimations on the remainder.

ii) Give the algorithm for the computation of the effective hamiltonian.

iii) Solve the evolution given by the effective hamiltonian (this is trivial in the non-resonant case i.e. when the effective hamiltonian acts in a one dimensional subspace).

In the present paper we shall solve, under appropriate conditions, the steps i) and ii). Our method is to generalise the time independent reduction scheme : first find perturbatively approximate "invariant subspaces" for the whole evolution and then to block diagonalise it using the transformation functions formalism [14, 15].

The content of the paper is at follows. Section II contains the general setting. The main technical results are contained in Section III, where the step i) above is solved. Section IV concerns the step ii). For the readers not interested in the mathematical details we give in Section V a short summary of the results and comment on some simple examples.

II. GENERAL SETTING

We consider a time dependent hamiltonian of the form

$$H(t) = H_0 + \lambda V(t) \tag{2.1}$$

where the unperturbed hamiltonian H_0 is self-adjoint with domain $\mathcal{D}(H_0)$ in the Hilbert space $\mathcal{H}$ of quantum states, and V(t) in a time dependent perturbation with coupling constant λ.

We assume that V(t) can be represented by the Fourier integral

$$V(t) = \int_{\Omega} d\omega \hat{V}(\omega)\, e^{-i\omega t} \tag{2.2}$$

where Ω is a set in $\mathbb{R}$ and $\hat{V}(\omega)$ is a measurable a.e. bounded operator valued function satisfying

$$\hat{V}^*(\omega) = \hat{V}(-\omega) \tag{2.3}$$

$$\int_{\Omega} d\omega\, |\omega|^k \| \hat{V}(\omega) \| < \infty, \qquad k = 0, 1 \tag{2.4}$$

All the results below hold true also for V(t) of the form

$$V(t) = f(t)V \tag{2.5}$$

with V a fixed bounded self-adjoint operator. The real valued function f(t) is the Fourier transform of a measure $d\mu(\omega)$

$$f(t) = \int_{\Omega} d\mu(\omega)\, e^{-i\omega t} \tag{2.6}$$

satisfying

$$\int_{\Omega} d\,|\mu(\omega)|\,|\omega|^k < \infty, \qquad k = 0, 1 \tag{2.7}$$

which can have pure point contributions at some specific frequencies. It follows from these assumptions that V(t) is uniformly bounded and norm differentiable. Although the proofs below make explicit use of the boundedness of V(t) (e.g. in writing down a Dyson expansion for the evolution operator) it is possible, at the expense of more technicalities, to extend the results of the present paper to some classes of unbounded time dependent perturbations.

Since V(t) is bounded and norm differentiable, H(t) is self-adjoint on $\mathcal{D}(H_0)$ and the evolution equation

$$i\frac{d}{dt}U(t, t_o) = H(t)\, U(t, t_o), \qquad U(t_o, t_o) = I \tag{2.8}$$

has a unique unitary solution [15]. We shall use the interaction picture

$$U_I(t, t_o) = e^{iH_o t}\, U(t, t_o)\, e^{-iH_o t} \tag{2.9}$$

with the equation of motion

$$i\frac{d}{dt}U_I(t, t_o) = \lambda\, H_I(t)\, U_I(t, t_o), \qquad U_I(t_o, t_o) = I \tag{2.10}$$

$$H_I(t) = e^{iH_o t}\, V(t)\, e^{-iH_o t} \tag{2.11}$$

As well known the solution of (2.10) can be represented, at any fixed time, by the norm convergent Dyson series

$$U_I(t, t_o) = I + \sum_{n=1}^{\infty} \lambda^n\, U_{I,\,n}(t, t_o) \tag{2.12}$$

with

$$U_{I,\,n}(t, t_o) = (-i)^n \int_{\Omega^n} d\omega^{(n)} \int_{t_o}^{t} ds_1 \int_{t_o}^{s_1} ds_2 \ldots \int_{t_o}^{s_{n-1}} ds_n$$

$$\exp\left(-i\sum_{j=1}^{n} \omega_j s_j\right) \hat{V}_I(\omega_1, s_1) \ldots \hat{V}_I(\omega_n, s_n) \tag{2.13}$$

where

$$d\omega^{(n)} = d\omega_1 \ldots d\omega_n$$

$$\hat{V}_I(\omega, t) = e^{iH_o t}\, \hat{V}(\omega)\, e^{-iH_o t} \tag{2.14}$$

and

$$\| U_{I,n}(t, t_o) \| \leq \frac{1}{n!}\left(\int_{\Omega} d\omega \,\| \hat{V}(\omega) \|\right)^n |t-t_o|^n \tag{2.15}$$

Introducing the adiabatic switching on of the interaction, i.e. replacing V(t) in (2.1) and (2.11) by $e^{\varepsilon t}\, V(t)$, one can push the initial time at infinity, $t_o = -\infty$. The evolution is again given by a norm convergent series

$$U_I^{\varepsilon}(t,-\infty) = I + \sum_{n=1}^{\infty} \lambda^n \; U_{I,n}^{\varepsilon}(t,-\infty) \tag{2.16}$$

$$U_{I,n}^{\varepsilon}(t,-\infty) = (-i)^n \int_{\Omega^n} d\omega^{(n)} \int_{-\infty}^{t} ds_1 \ldots \int_{-\infty}^{s_{n-1}} ds_n \exp\left(-i \sum_{j=1}^{n} (\omega_j + i\varepsilon)s_j\right) \prod_{j=1}^{n} \hat{V}_I(\omega_j, s_j) \tag{2.17}$$

$$\| U_{I,n}^{\varepsilon}(t,-\infty) \| \leq \frac{1}{n!} \left(\frac{e^{\varepsilon t}}{\varepsilon} \int_{\Omega} d\omega \, \| \hat{V}(\omega) \| \right)^n \tag{2.18}$$

Note that , while norm convergent for $\varepsilon > 0$, the terms of the series (2.16) can blow up as $\varepsilon \to 0$, so (2.16) has no meaning in the limit $\varepsilon \to 0$. Alternatively each term in (2.12) is, in general, of order $\lambda^n (t - t_o)^n$, so in the limit $t - t_o \to \infty$, not only the series become divergent but each term becomes infinite.

The main point of this paper in that (under appropriate circumstances) the situation is better when one considers the evolution of orthogonal projections (i.e. subspaces). Let $P(t_o)$ be the orthogonal projection on some subspace of initial states in $\mathcal{H}$; then its time evolution is given by

$$P(t) = U(t, t_o)\, P(t_o)\, U^*(t, t_o) \tag{2.19}$$

In the interaction picture, one has

$$P_I(t) = U_I(t, t_o)\, P_I(t_o)\, U_I^*(t, t_o) \tag{2.20}$$

where

$$P_I(t) = e^{iH_o t}\, P(t)\, e^{-iH_o t} \tag{2.21}$$

Due to (2.12), $P_I(t)$ has a perturbation expansion

$$P_I(t) = P_I(t_o) + \sum_{n=1}^{\infty} \lambda^n P_{I,n}(t) \tag{2.22}$$

$$P_{I,n}(t) = \sum_{k=0}^{n} U_{I,k}(t, t_o)\, P_I(t_o)\, U_{I,n-k}^{*}(t, t_o) \tag{2.23}$$

The fact that $P_I(t)$ is a projection implies that

$$P_{I,n}(t) = \sum_{k=0}^{n} P_{I,k}(t)\, P_{I,n-k}(t) \tag{2.24}$$

In the adiabatic switching on scheme the formulae (2.22)-(2.24) have the form

$$P_I^{\varepsilon}(t) = P_o + \sum_{n=1}^{\infty} \lambda^n P_{I,n}^{\varepsilon}(t) \tag{2.25}$$

where P_o stands for $P_I(-\infty)$,

$$P_{I,n}^{\varepsilon}(t) = \sum_{k=0}^{n} U_{I,k}^{\varepsilon}(t,-\infty)\, P_o\, U_{I,n-k}^{\varepsilon *}(t,-\infty) \tag{2.26}$$

$$P_{I,n}^{\varepsilon}(t) = \sum_{k=0}^{n} P_{I,k}^{\varepsilon}(t)\, P_{I,n-k}^{\varepsilon}(t) \tag{2.27}$$

The estimations (2.15) and (2.18) give the obvious estimations for $P_{I,n}(t)$ and $P_{I,n}^{\varepsilon}(t)$

$$\| P_{I,n}(t) \| \leq \frac{1}{n!} \left(2|t-t_o| \int_{\Omega} d\omega \, \| \hat{V}(\omega) \| \right)^n$$

$$\| P_{I,n}^{\varepsilon}(t) \| \leq \frac{1}{n!} \left(\frac{2e^{\varepsilon t}}{\varepsilon} \int_{\Omega} d\omega \, \| \hat{V}(\omega) \| \right)^n \tag{2.28}$$

which again blow up when $|t-t_o| \to \infty$ or $\varepsilon \to 0$.

III. UNIFORM ESTIMATES IN TIME

In this section, we show that provided the initial condition $P_I(t_o)$ is suitable chosen and n is not too large, $P_{I,n}(t)$ are uniformly bounded in time.

We assume that the spectrum $\sigma(H_o)$ of the unperturbed hamiltonian has a bounded isolated part σ_o, with P_o the corresponding spectral projection

$$P_o = \frac{i}{2\pi} \oint_\Gamma dz\, R(z), \qquad R(z) = (H_o - z)^{-1} \tag{3.1}$$

where Γ is a contour in the complex z-plane enclosing σ_o, but none of the points of the complement σ_1 of σ_o in $\sigma(H_o)$. Let

$$d = \text{dist}(\sigma_o, \sigma_1) > 0$$

and for any complex number u, denote by

$$\sigma_j(u) = \{E + u \mid E \in \sigma_j\}, \qquad j = 0, 1$$

the translates of the sets σ_o and σ_1 by u. For $\omega^{(n)} = \{\omega_1, ..., \omega_n\} \in \Omega^n$ and $\varepsilon > 0$, define the sets

$$\sum_j (\omega^{(n)}, \varepsilon) = \bigcup_{m=1}^{n} \sigma_j\left(-\sum_{k=m}^{n} \omega_k - i\,(n - m + 1)\,\varepsilon\right) \cup \sigma_j, \qquad j = 0, 1 \tag{3.2}$$

Note that

$$\text{dist}\left(\sum_o (\omega^{(n)}, \varepsilon), \sum_1 (\omega^{(n)}, \varepsilon)\right) \geq \min(\varepsilon, d) \tag{3.3}$$

Let $\Gamma(\omega^{(n)}, \varepsilon)$ be a contour which encloses $\sum_o (\omega^{(n)}, \varepsilon)$, but contains no points of $\sum_1 (\omega^{(n)}, \varepsilon)$.

Proposition 1

Let $P^{\varepsilon}_{I,n}(t)$ be given by (2.26) with P_o given by (3.1). Then

$$P^{\varepsilon}_{I,n}(t) = (-1)^n e^{iH_o t} \left[\int_{\Omega^n} d\omega^{(n)} \exp\left(-it \sum_{j=1}^{n} (\omega_j + i\varepsilon)\right) \right.$$

$$\left. \frac{i}{2\pi} \oint_{\Gamma(\omega^{(n)}, \varepsilon)} dz \left\{ \prod_{m=1}^{n} R\left(z + \sum_{j=m}^{n} \omega_j + i\,(n - m + 1)\,\varepsilon\right) \hat{V}(\omega_m) \right\} R(z) \right] e^{-iH_o t} \tag{3.4}$$

Proof :

After the change of variables $s_m = \sum_{j=1}^{m} t_j$, $m = 1, ..., n$, (2.17) becomes

$$U^{\varepsilon}_{I,n}(t,-\infty) = (-i)^n \int_{\Omega^n} d\omega^{(n)} \int_{-\infty}^{t} dt_1 \int_{-\infty}^{o} dt_2 \ldots \int_{-\infty}^{o} dt_{n-1} \int_{-\infty}^{o} dt_n$$

$$\left\{ \prod_{m=1}^{n} \exp\left[it_m \left(H_o - \sum_{j=m}^{n} (\omega_j + i\varepsilon) \right) \right] \hat{V}(\omega_m) \right\} \exp\left[-iH_o \sum_{j=1}^{n} t_j \right] \tag{3.5}$$

We now consider the k^{th} term of the sum (2.26), k = 0, 1, ..., n, and label the n-k integration variables occuring in $U^{\varepsilon *}_{I,n-k}(t,-\infty)$ as $\omega_n, \omega_{n-1},\ldots,\omega_{k+1}$ and $t_n, t_{n-1}, \ldots, t_{k+1}$. Hence

$$U^{\varepsilon}_{I,k}(t,-\infty)\, P_o\, U^{\varepsilon *}_{I,n-k}(t,-\infty) = i^n(-1)^k \int_{\Omega_n} d\omega^{(n)} \int_{-\infty}^{t} dt_1 \int_{-\infty}^{o} dt_2 \ldots \int_{-\infty}^{o} dt_{n-1} \int_{-\infty}^{t} dt_n$$

$$\left\{ \prod_{m=1}^{k} \exp\left[it_m \left(H_o - \sum_{j=m}^{k} (\omega_j + i\varepsilon) \right) \right] \hat{V}(\omega_m) \right\} \left\{ \exp\left[-iH_o \sum_{j=1}^{k} t_j \right] P_o \exp\left[iH_o \sum_{j=k+1}^{n} t_j \right] \right\}$$

$$\left\{ \prod_{m=k+1}^{n} \hat{V}^*(\omega_m) \exp\left[-it_m \left(Ho - \sum_{j=k+1}^{m} (\omega_j - i\varepsilon) \right) \right] \right\} \tag{3.6}$$

The spectral theorem for H_o allows to write the second bracket in (3.6) as the spectral integral

$$\int_{\sigma_o} dP(E) \exp\left[-iE \left(\sum_{j=1}^{k} t_j - \sum_{j=k+1}^{n} t_j \right) \right] \tag{3.7}$$

where P(E) is the spectral measure of H_o. Introducing (3.7) in (3.6) and permuting the spectral with the time integrals (Fubini's theorem), one can perform the time integrations with the help of the Laplace transform

$$\int_{-\infty}^{t} ds \exp\left[is(H_o - \omega - i\varepsilon) \right] = -i\, R(\omega + i\varepsilon) \exp\left[it(H_o - \omega - i\varepsilon) \right], \quad \varepsilon > 0 \tag{3.8}$$

This leads to

$$U^{\varepsilon}_{I,k}\ (t, -\infty)\ P_0\ U^{\varepsilon *}_{I,n-k}\ (t, -\infty) =$$

$$= (-1)^n\, e^{iH_0 t} \int_{\Omega^n} d\omega^{(n)} \int_{\sigma_0} \exp\left[-it \left(\sum_{j=1}^{k} (\omega_j + i\varepsilon) - \sum_{j=k+1}^{n} (\omega_j - i\varepsilon) \right) \right]$$

$$\left\{ \prod_{m=1}^{k} R\left(E + \sum_{j=m}^{k} \omega_j + i\,(k - m + 1)\varepsilon \right) \hat{V}(\omega_m) \right\} dP(E)$$

$$\left\{ \prod_{m=k+1}^{n} \hat{V}^*(\omega_m)\, R^*\left(E + \sum_{j=k+1}^{m} \omega_j + i\,(m-k)\,\varepsilon \right) \right\} e^{iH_0 t} \qquad (3.9)$$

In order to establish the validity of (3.4), we note that, for a fixed $\omega^{(n)}$, the integrand in (3.4) is holomorphic except on the $n + 1$ disjoint sets σ_0 and $\sigma_0\left(-\sum_{j=m}^{n} \omega_j - i\,(n - m + 1)\,\varepsilon \right)$, $m = 1, \ldots, n$. Thus we can deform the contour $\Gamma(\omega^{(n)}, \varepsilon)$ (see formula (3.4)) into $n + 1$ subcontours Γ_{n-k}, $k = 0, \ldots, n$, with Γ_{n-k} enclosing $\sigma_0\left(-\sum_{j=k+1}^{n} \omega_j - i\,(n - k)\,\varepsilon \right)$, $k = 0, 1, \ldots n-1$, and Γ_0 enclosing σ_0. In particular, all resolvents occuring in (3.4) are holomorphic in Γ_{n-k} except for

$$R\left(z + \sum_{j=k+1}^{n} \omega_j - i\,(n - k)\,\varepsilon \right) = \int_{\mathbb{R}} dP(E)\, \frac{1}{E - \sum_{j=k+1}^{n} \omega_j - i\,(n - k)\,\varepsilon - z} \qquad (3.10)$$

Therefore the contribution of Γ_{n-k} to the contour integral is of the form

$$\frac{i}{2\pi}\oint_{\Gamma_{n-k}} dz\, A(z)\, R\left(z+\sum_{j=k+1}^{n}\omega_j - i(n-k)\varepsilon\right) B(z)$$

$$=\frac{i}{2\pi}\int_{\mathbb{R}}\oint_{\Gamma_{n-k}} dz\, \frac{A(z)\, dP(E)\, B(z)}{E-\sum_{j=k+1}^{n}\omega_j - i(n-k)\varepsilon - z}$$

$$=\int_{\sigma_o} A\left(E-\sum_{j=k+1}^{n}\omega_j - i(n-k)\varepsilon\right) dP(E)\, B\left(E-\sum_{j=k+1}^{n}\omega_j - i(n-k)\varepsilon\right) \qquad (3.11)$$

where A(z) and B(z) are holomorphic in Γ_{n-k}. In the proof of (3.11), the contour and spectral integrals have been permuted. The spectral integral can be restricted to σ_o since in Γ_{n-k}, the integrand of the r.h.s. of (3.11) is holomorphic when E does not belong to σ_o. Using this result in (3.4), changing the signs of the dummy variables ω_j, $j = k+1, \ldots, n$, recalling that $\hat{V}^*(\omega) = \hat{V}(-\omega)$ and $R^*(z) = R(z^*)$, one sees that the contribution of Γ_{n-k}, $k = 0, 1, \ldots, n$, to (3.4) is just (3.9). Summing up these contributions leads to the formula (3.4).

The result in proposition 1 is general, in particular it does not depend on any assumption on the nature of the frequency spectrum of the time dependent perturbation V(t). Note that in view of (3.3) it is possible to choose a contour $\Gamma(\omega^{(n)}, \varepsilon)$ which is at least at distance $\min\left\{\frac{\varepsilon}{2}, \frac{d}{2}\right\}$ from $\sum_o(\omega^{(n)}, \varepsilon)$ and $\sum_1(\omega^{(n)}, \varepsilon)$. Hence all resolvents in (3.4) are bounded by $2/\varepsilon$ (for ε small), which gives an estimate of the form (2.28), useless in the limit $\varepsilon \to 0$.

The proposition 2 below shows, however, that as long as σ_o is not resonant (through the frequency spectrum of V(t) and its harmonics) with σ_1, the projection $P^{\varepsilon}_{I,n}(t)$ have limits as $\varepsilon \to 0$ which are uniformly bounded in t. For this we set $d_o = d$ and

$$d_n = \inf_{\omega^{(n)} \in \Omega^n} \operatorname{dist}\left(\sum_o(\omega^{(n)}), \sum_1(\omega^{(n)})\right), \quad n = 1, 2, \ldots \qquad (3.12)$$

with $\sum_r(\omega^{(n)}) = \sum_r(\omega^{(n)}, \varepsilon = 0)$, $r = 1, 2$. Observe that $d_{n+1} \leq d_n$.

Proposition 2

Let N be the smallest positive integer such that $d_{N+1} = 0$ and for $\omega^{(n)} \in \Omega^n$, $n \leq N$, let $\Gamma(\omega^{(n)})$ be a contour enclosing $\sum_0(\omega^{(n)})$ but no points of $\sum_1(\omega^{(n)})$. Then for $1 \leq n \leq N$

$$P_{I,n}(t) = \text{norm} - \lim_{\varepsilon \to 0} P^{\varepsilon}_{I,n}(t) \tag{3.13}$$

exist and

$$P_{I,n}(t) = (-1)^n e^{iH_0 t}\left[\int_{\Omega^n} d\omega^{(n)} \exp\left(-it\sum_{j=1}^{n}\omega_j\right)\right.$$

$$\left.\frac{i}{2\pi}\oint_{\Gamma(\omega^{(n)})} dz\left\{\prod_{m=1}^{n} R(z+\sum_{j=m}^{n}\omega_j)\,\hat{V}(\omega_m)\right\}R(z)\right] e^{-iH_0 t} \tag{3.14}$$

$$P_{I,n}(t) = \sum_{k=0}^{n} P_{I,k}(t)\,P_{I,n-k}(t), \qquad 1 \leq n \leq N \tag{3.15}$$

$$i\frac{d}{dt}P_{I,n}(t) = \left[H_I(t), P_{I,n-1}(t)\right], \qquad 1 \leq n \leq N \tag{3.16}$$

with

$$P_{I,0}(t) = P_0 \tag{3.17}$$

$$\| P_{I,n}(t) \| \leq C_1\left(\frac{2}{d_n}\right)^{n+1} v^n \tag{3.18}$$

where

$$v = \int_{\Omega} (1 + |\omega|)\, \| \hat{V}(\omega) \|\, d\omega$$

Proof :

Notice that the definition of the sets (3.2) together with (3.12) imply that

$$\inf_{\omega^{(n)} \in \Omega^n} \operatorname{dist}\left(\sum_0 (\omega^{(n)}, \varepsilon) , \sum_1 (\omega^{(n)}, \varepsilon) \right) \geq d_n \geq d_N \tag{3.19}$$

for all $\varepsilon > 0$ and $n \leq N$. Thus it is possible to find a contour $\Gamma(\omega^{(n)})$ independent of $\varepsilon \in [0, \varepsilon_0]$, which encloses the sets $\sum_0 (\omega^{(n)}, \varepsilon)$ but no points of the sets $\sum_1 (\omega^{(n)}, \varepsilon)$, such that (see Fig. 1 for an illustrative simple case)

$$\operatorname{dist}\left(\Gamma(\omega^{(n)}), \sum_0 (\omega^{(n)}, \varepsilon) \cup \sum_1 (\omega^{(n)}, \varepsilon) \right) \geq \frac{d_n}{2} \tag{3.20}$$

and

$$\text{length } \Gamma(\omega^{(n)}) \leq 2\left(C + \sum_{k=1}^{n} |\omega_k| \right) \leq 2\,(1 + C) \prod_{k=1}^{n} \left(1 + |\omega_k|\right) \tag{3.21}$$

with $C = n\,\varepsilon_0 + 2\,d_n + \operatorname{diam} \sigma_0$.

We use $\Gamma(\omega^{(n)})$ in (3.4) and let $\varepsilon \to 0$. The resolvents converge in norm to their corresponding limits, and so does $P^{\varepsilon}_{I,n}(t)$. This proves (3.14). The relation (3.15) follows immediately from the corresponding relation (2.27).

From (2.26) it follows that $P^{\varepsilon}_{I,n}(t)$ is differentiable and

$$i \frac{d}{dt} P^{\varepsilon}_{I,n}(t) = e^{\varepsilon t} \left[H_I(t) , P^{\varepsilon}_{I,n-1}(t) \right], \qquad n = 1, 2, \ldots$$

whereof (3.16) follows. Taking into account (3.2), the norms of all the resolvents appearing in (3.14) are less than $2/d_n \leq 2/d_N$ which together with (3.21) gives (3.18) with $C_1 = (1 + C)/\pi$.

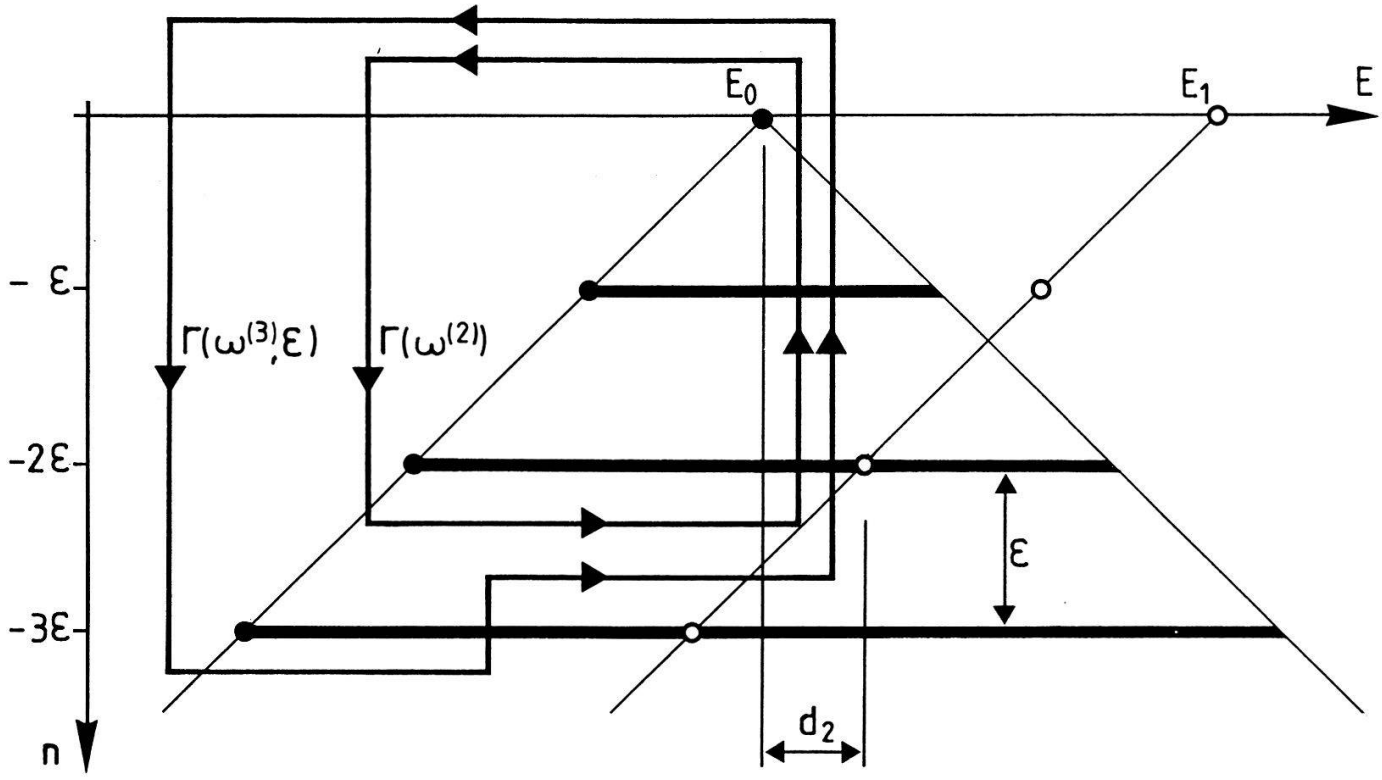

Figure 1

$\sigma_o = \{E_o\}$ and $\sigma_1 = \{E_1\}$ consist of the two isolated points E_o and E_1 with $d = E_1 - E_o > 0$. The perturbation has a continuous range of frequencies with support $\Omega = [-\omega_o, \omega_o]$. One has $d_n = d - n\omega_o$, and in the case of the figure, N = integer part of $d/\omega_o = 2$. The solide horizontal lines represent the sets of translates $\{E_o + n\omega - in\varepsilon, \omega \in [-\omega_o, \omega_o]\}$ of σ_o. With the choice $\omega^{(n)} = \{-\omega_o, -\omega_o, ..., -\omega_o\}$, the black points $E_o - k\omega_o - ik\varepsilon$ (resp white points $E_1 - k\omega_o - ik\varepsilon$), k = 0, 1, ..., n, belong to $\sum_o(\omega^{(n)}, \varepsilon)$ (resp. $\sum_1(\omega^{(n)}, \varepsilon)$). The contour $\Gamma(\omega^{(3)},\varepsilon)$ occurs in the expression (3.4) of $P^{\varepsilon}_{I,3}(t)$ (proposition 1). The contour $\Gamma(\omega^{(2)})$, which is used in the definition (3.14) of $P_{I,2}(t)$ (proposition 2), can be fixed independently of ε as $\varepsilon \to 0$.

Remarks

i) By inspection one can see that there is an alternative formula for d_n

$$d_n = \inf\left\{ \left| E_i - E_f - \sum_{j=1}^{m} \omega_j \right|, \left| E_i - E_f \right| \right\}$$

where the infimum is taken over all $E_i \in \sigma_0$, $E_f \in \sigma_1$, $\omega_j \in \Omega$ and $1 \leq m \leq n$. This is nothing but the usual "nonresonance" condition of the usual perturbation theory. In general, N is some finite positive integer. For instance if $\Omega = [-\omega_0, \omega_0]$ with $0 < \omega_0 < d$, then $d_n = d - n\,\omega_0$, so N is the largest integer such that $N < d/\omega_0$.

ii) Consider now the situation when $V(t) = V \cos \omega_0 t$. In this case it may happen that $d_n > d_\infty > 0$ and then the series for $P_I(t)$ converge for λ small enough (the simplest example in that of a two level atom with energies E_0, E_1 such that $|E_1 - E_0| \neq k\omega_0$ for all $k = 0, 1, \ldots$). A more interesting case is a two level atom with $V(t) = \sum_{j=1}^{p} V_j \cos \omega_j t$. In this case one may still have $d_n > 0$ for all $n \geq 0$. In this case the convergence of the series for $P_I(t)$ is a more delicate matter and we will consider it in a future work.

iii) Convergence is always achieved in the static case which corresponds to set $\omega_0 = 0$ in the situation described above. In this case (going back to the Schrödinger picture) (3.14) reduces to

$$P_n = (-1)^n \frac{i}{2\pi} \oint_\Gamma dz\, (R(z)V)^n R(z) \tag{3.22}$$

which is nothing but the usual time independent perturbation formula [14]. Notice that for given n the formula (3.14) goes smoothly to (3.22) as $\omega_0 \to 0$. Let us point out finally that the method of computing $P_{I,n}(t)$ in propositions 1 and 2 is the generalisation to the time dependent case of the proof in [16] of the Gell-Mann-Low formula. One can also prove proposition 2 by checking directly that the expressions (3.14) for the $P_{I,n}(t)$ fullfil the recursion relations (3.15) and (3.16).

iv) The limit of $P_{I,n}^{\varepsilon}(t)$ as $\varepsilon \to 0$ can exist even if $n > N$, but it will no more be given by the formula (3.14). This may arise, for instance, for transitions from bound to ionized states when σ_1 is absolutely continuous. The limit may also exists when the frequency distribution $\hat{f}(\omega)$ is sufficiently smooth. An elementary example of the latter case is given in Section V. We shall come back to these more general situations in future work.

The above results show that, provided proper initial conditions at $t_o = -\infty$ are chosen, the Gell-Mann-Low switching procedure leads to expansions in the coupling constant whose coefficients are uniformly bounded in t up to some order. The next step is to obtain similar results for finite time initial conditions. The need for that is obvious from the physical point of view; for example it will not be possible to describe the Rabi oscillations [13] in the Gell-Mann-Low formalism: during the infinite interval of time from $-\infty$ to 0 the radiative damping, albeit small, will decay completely the bound states.

The problem is how to chose $P_I(t_o)$, in order to ensure that its evolution given by (2.20) has an expansion in λ up to order N with uniformly bounded coefficients and a small reminder. Notice that one cannot follow simply the naive extension of the Gell-Mann-Low theorem

$$P_I(t_o) = \lim_{\varepsilon \to 0} P_I^{\varepsilon}(t_o) \tag{3.23}$$

since, at the present stage, we have proved that the limit exists only for the first N coefficients; in particular the limit in (3.23) may not exists. Also one cannot take (see proposition 2)

$$P_I(t_o) = \sum_{j=0}^{N} \lambda^j P_{I,j}(t_o) \tag{3.24}$$

since the truncated series in the r.h.s. of (3.24) does not represent a projection. So the natural thing to do is to seek the following form for $P_I(t_o)$

$$P_I(t_o) = \tilde{P}_I(t_o) = \sum_{j=0}^{N} \lambda^j P_{I,j}(t_o) + \lambda^{N+1} R_I(t_o, \lambda) \tag{3.25}$$

and to provide suitable estimates on the remainder $R_I(t_o, \lambda)$. We shall use the following simple perturbation lemma.

Lemma 1.

Let $0 \leq \delta \leq 3/16$ and T be a bounded self-adjoint operator satisfying $\| T^2 - T \| \leq \delta$. Then

i) $\sigma(T) \subset [-2\delta, 2\delta] \cup [1-2\delta, 1 + 2\delta]$

ii) the spectral projection of T corresponding to $[1-2\delta, 1+ 2\delta]$, i.e.

$$P = \frac{i}{2\pi} \oint_{|z-1|=1/2} dz\,(T-z)^{-1}\,, \text{ satisfies } \|T - P\| \leq 2\delta.$$

Proof

i) From the functional calculus

$$\sup_{\lambda \in \sigma(T)} |\lambda^2 - \lambda| = \|T^2 - T\| \leq \delta$$

Hence $\sigma(T) \subset \{\lambda\,;\, |\lambda^2 - \lambda| \leq \delta\}$.

ii) Write $T = PTP + (1 - P)\,T\,(1 - P)$ (recall that $[P, T] = 0$), so that $T - P = P\,(T - 1)\,P + (1 - P)\,T\,(1 - P)$ and then

$$\|T - P\| \leq \max\left\{ \|P(T - 1)\,P\|,\ \|(1 - P)\,T\,(1 - P)\| \right\}$$

Now use the fact that $\sigma(P(T - 1)P) \subset [-2\delta, 2\delta]$, $\sigma((1 - P)\,T\,(1 - P)) \subset [-2\delta, 2\delta]$ and again the function calculus.

Consider, for $t \in \mathbb{R}$

$$T_N(t) = Po + \sum_{j=1}^{N} \lambda^j P_{I,j}(t) \tag{3.26}$$

Since $P_{I,j}(t)$ obey the relations (3.15) one has

$$T_N^2(t) - T_N(t) = \sum_{k=N+1}^{2N} \lambda^k \sum_{\substack{0 \leq l\,,\, m \leq N \\ l + m = k}} P_{I,l}(t)\, P_{I,m}(t) \tag{3.27}$$

whereof, by (3.18), for every $\lambda_1 > 0$ there exists $A < \infty$ (A independent of t), such that

$$\|T_N^2(t) - T_N(t)\| \leq \lambda^{N+1} A, \qquad 0 \leq \lambda \leq \lambda_1 \tag{3.28}$$

For sufficiently small λ one can apply the lemma 1 and define

$$\tilde{P}_I(t) = \frac{i}{2\pi} \oint_{|z-1|=1/2} dz\, (T_N(t) - z)^{-1} \tag{3.29}$$

We conclude from the lemma 1 and the fact that the estimate (3.28) is uniform in t that $\tilde{P}_I(t)$ is indeed of the form (3.25) with $\| R_I(\lambda, t) \| \leq C$ where C is independent of t and λ. We will simply write the expansion

$$\tilde{P}_I(t) = \sum_{j=0}^{N} \lambda^j P_{I,j}(t) + O(\lambda^{N+1}) \tag{3.30}$$

where $O(\lambda^{N+1})$ means an operator whose norm is bounded by const. λ^{N+1} uniformly in time.

The result below shows in particular that $\tilde{P}_I(t_o)$ has all the properties we required for a "good" initial condition.

Proposition 3

$$i \frac{d}{dt} \tilde{P}_I(t) = \lambda \left[H_I(t), \tilde{P}_I(t) \right] + \lambda^{N+1} S(t, \lambda) \tag{3.31}$$

where

$$S(t, \lambda) = \frac{i}{2\pi} \oint_{|z-1|=1/2} dz\, (T_N(t) - z)^{-1} \, [H_I(t), P_{I,N}(t)] \, (T_N(t) - z)^{-1} \tag{3.32}$$

$$\| \tilde{P}_I(t) - U_I(t, t_o) \tilde{P}_I(t_o) \, U_I^*(t, t_o)) \| \leq \lambda^{N+1} \int_{t_o}^{t} du \, \| S(u, \lambda) \| \tag{3.33}$$

Proof

From (3.29), (3.26) and (3.16)

$$i\frac{d}{dt}\tilde{P}_I(t) = -\frac{i}{2\pi}\oint_{|z-1|=1/2} dz\ (T_N(t)-z)^{-1}\left(i\frac{d}{dt}T_N(t)\right)(T_N(t)-z)^{-1} =$$

$$= -\frac{i}{2\pi}\oint_{|z-1|=1/2} dz\,(T_N(t)-z)^{-1}\left\{\lambda\left[H_I(t), T_N(t)-z\right] - \right.$$

$$\left. - \lambda^{N+1}\left[H_I(t), P_{I,N}(t)\right]\right\}(T_N(t)-z)^{-1}$$

whereof (3.31) and (3.32) follow. Denoting

$$\Delta P(t) = \tilde{P}_I(t) - U_I(t, t_o)\,\tilde{P}_I(t_o)\,U_I^*(t, t_o)$$

one has

$$i\frac{d}{dt}\Delta P(t) = \lambda\,[H_I(t), \Delta P(t)] + \lambda^{N+1}\,S(t, \lambda)$$

whereof

$$i\frac{d}{dt}\left(U_I^*(t, t_o)\,\Delta P(t)\,U_I(t, t_o)\right) = \lambda^{N+1}\,U_I^*(t, t_o)\,S(t, \lambda)\,U_I(t, t_o)$$

which gives (3.33).

The remainder $S(t, \lambda)$ in (3.31) is also uniformly bounded in time since all operators occuring in (3.32) have this property. Thus proposition 3 implies

$$\tilde{P}_I(t) = U_I(t, t_o)\,\tilde{P}_I(t_o)\,U_I^*(t, t_o) + O\left(\lambda^{N+1}|t-t_o|\right) \tag{3.34}$$

IV. REDUCTION THEORY AND THE EFFECTIVE HAMILTONIAN

In this section, using the results of the previous one, we shall perform the reduction scheme generalizing the time independent procedure. As in the time independent case we use the transformation function method ([14], Chap. II, § 4).

Consider the pair of orthogonal projections P_o, $\tilde{P}_I(t)$ where $\tilde{P}_I(t)$ is defined in (3.29). By (3.30), one can find λ_o (independent of t) such that

$$\| P_o - \tilde{P}_I(t) \| < 1 \qquad |\lambda| \leq \lambda_o \ . \tag{4.1}$$

Therefore P_o and $\tilde{P}_I(t)$ are unitarily equivalent for all times, i.e., there exists a unitary operator $M_I(t)$ (the transformation function) such that

$$\tilde{P}_I(t) = M_I(t)\ P_o\ M_I^*(t), \qquad M_I^{-1}(t) = M_I^*(t) \tag{4.2}$$

The transformation function is clearly not unique. If $K(t)$ is any unitary transformation such that $[K(t), P_o] = 0$, then the product $M_I(t)\ K(t)$ also satisfies (4.1).

As explained in the introduction, we want to factorize in the total evolution phase factors having an unbounded growth in time from a part which remains bounded in time when expanded in powers of λ. We require that the transformation function $M_I(t)$ has the latter property : $M_I(t)$ should have an expansion in λ up to order N with coefficients bounded in time. Moreover, $M_I(t)$ should reduce to the identity when $\lambda \to 0$. The transformation function defined by Sz.-Nagy

$$M_I(t) = \left(1 - (\tilde{P}_I(t) - P_o)^2\right)^{-1/2} \left[\tilde{P}_I(t)\ P_o + (I - \tilde{P}_I(t)\ (I-P_o))\right] \tag{4.3}$$

is a convenient choice for two reasons. Since it is an algebraic expression in $\tilde{P}_I(t)$, it can easily be expanded; moreover the coefficients will have the requested boundness property (see (4.8) below).

Then one can define the "rotated" evolution

$$W_I(t, t_o) = M_I^*(t)\ U_I(t, t_o)\ M_I(t_o) \tag{4.4}$$

The equation of motion for $W_I(t, t_o)$ follows from (4.4) and (2.10)

$$i \frac{d}{dt} W_I(t, t_o) = H_I^{ef}(t)\ W_I(t, t_o) \tag{4.5}$$

where the effective hamiltonian (in the interaction picture) is given by

$$H_I^{ef}(t) = \lambda M_I^*(t)\ H_I(t)\ M_I(t) \ - i\ M_I^*(t) \frac{d}{dt} M_I(t) \tag{4.6}$$

We now come to the perturbation expansions for $M_I(t)$ and $H_I^{ef}(t)$. When (4.1) holds, $\left(I - (\tilde{P}_I(t) - P_o)^2\right)^{-1/2}$ is represented for all times by the convergent series

$$\left(I - (\tilde{P}_I(t) - P_o)^2\right)^{-1/2} = I + \sum_{j=1}^{\infty} \frac{(2j-1)!!}{j!\, 2^j} (\tilde{P}_I(t) - P_o)^{2j} \tag{4.7}$$

Using (4.7) in (4.3) together with the expansion (3.30) of $\tilde{P}_I(t)$ leads to the expansion of $M_I(t)$

$$M_I(t) = I + \sum_{j=1}^{N} \lambda^j M_{I,j}(t) + O(\lambda^{N+1}) \tag{4.8}$$

Since the $M_{I,j}(t)$ are expressed by the $P_{I,k}(t)$, $k = 1,\ldots, j$, they are uniformly bounded in t. (see formula (4.19) below for the first terms). As in (3.30), $O(\lambda^{N+1})$ represents an operator with norm bounded by const. λ^{N+1} uniformly in time. It follows from the proposition 3, (3.30) and (3.16) that

$$\frac{d}{dt}\tilde{P}_I(t) = \sum_{j=1}^{N} \lambda^j \frac{d}{dt} P_{I,j}(t) + O(\lambda^{N+1}) \tag{4.9}$$

where $O(\lambda^{N+1})$ is again uniform in t. This implies with (4.3) and (4.7) that

$$\frac{dM_I(t)}{dt} = \sum_{j=1}^{N} \lambda^j \frac{d}{dt} M_{I,j}(t) + O(\lambda^{N+1}) \tag{4.10}$$

where $\frac{d}{dt} M_{I,j}(t)$ are uniformly bounded.

With this we can state the properties of the expansion of $H_I^{ef}(t)$:

Proposition 4

The effective hamiltonian (4.6) has an expansion up to order N

$$H_I^{ef}(t) = \sum_{j=1}^{N} \lambda^j H_{I,j}^{ef}(t) + O(\lambda^{N+1}) \tag{4.11}$$

with the following properties

i) the operators $H^{ef}_{I,j}(t)$, j = 1, ..., N, as well as the remainder $O(\lambda^{N+1})$ are uniformly bounded in t.

ii) $H^{ef}_{I,j}(t)$ are reduced by the subspace P_o, i.e.

$$\left[H^{ef}_{I,j}(t), P_o\right] = 0 \qquad j = \quad , \quad 1, \ldots, N$$

Proof :

The existence of the expansion (4.11) and of i) follow immediately from (4.6), (4.8) and (4.10). To show ii), we first differentiate (4.2) with respect to t

$$i\frac{d\tilde{P}_I(t)}{dt} = i\left(\frac{dM_I(t)}{dt} P_o M_I^*(t) + P_o M_I(t) \frac{dM_I^*(t)}{dt}\right) =$$

$$= \left[i\frac{dM_I(t)}{dt} M_I^*(t), \tilde{P}_I(t)\right] \tag{4.12}$$

To obtain (4.12) we have used (4.2) again and $\frac{d}{dt}\left(M_I(t) M_I^*(t)\right) = 0$. Comparing (4.12) with (3.31) leads to

$$\left[\lambda H_I(t) - i\frac{dM_I(t)}{dt} M_I^*(t), \tilde{P}_I(t)\right] = O(\lambda^{N+1}) \tag{4.13}$$

Since M(t) is unitary (see (4.2)), this is equivalent with

$$\left[\lambda M_I^*(t) H_I(t) M_I(t) - i M_I^*(t) \frac{dM_I(t)}{dt}, P_o\right] = \left[H_I^{ef}(t), P_o\right] = O(\lambda^{N+1}) \tag{4.14}$$

The result ii) follows from (4.11) and (4.14).

For practical purposes, one will calculate $H_I^{ef}(t)$ up to a certain order $q \leq N$, setting

$$H^{ef\,q}_I(t) = \sum_{j=1}^{q} \lambda^j H^{ef}_{I,j}(t) \tag{4.15}$$

and $W_I^q(t, t_o)$ the corresponding "rotated" evolution

$$i\frac{d}{dt}\, W_I^q(t, t_o) = H_I^{ef\,q}(t)\, W_I^q(t, t_o) \tag{4.16}$$

The main point is that $H_I^{ef\,q}(t)$ commutes with P_o, so the equation (4.16) can be integrated separately in $P_o \mathcal{H}$ and in $(I-P_o)\mathcal{H}$. Usually, in practice, $P_o \mathcal{H}$ is a finite dimensional subspace, so the problem is reduced there to a finite system of first order differential equations.

The error made can be estimated from a comparison of (4.5) and (4.16) and the fact that $H_I^{ef}(t) = H_I^{ef\,q}(t) + O(\lambda^{q+1})$. Indeed

$$i\frac{d}{dt}\left(W_I^{q^*}(t, t_o)\, W_I(t, t_o)\right) = W_I^{q^*}(t, t_o)\, \left(H_I^{ef}(t) - H_I^{ef\,q}(t)\right)\, W_I(t, t_o)$$

leads at once to the estimate

$$\begin{aligned} \| W_I(t, t_o) - W_I^q(t, t_o) \| &= \| W_I^{q^*}(t, t_o)\, W_I(t, t_o) - I \| \\ &\leq \int_{t_o}^{t} ds\, \| H_I^{ef}(s) - H_I^{ef\,q}(s) \| = O\left(\lambda^{q+1} |t-t_o|\right) \end{aligned} \tag{4.17}$$

Since $M_I(t)$ is unitary we have obviously the same estimate for the complete evolution

$$\| U_I(t, t_o) - M_I(t)\, W_I^q(t,t_o)\, M_I^*(t_o) \| = O\left(\lambda^{q+1} |t-t_o|\right) \tag{4.18}$$

Of course, a knowledge of $U_I(t, t_o)$ requires also that of $M_I(t)$, which can be calculated from (4.8) to a given order less than N, as well as that of $W_I^q(t, t_o)$ in the complementary subspace $(I - P_o)\mathcal{H}$. In practice, relevant information can already be obtained from the sole knowledge of the "rotated" evolution restricted to the subspace $P_o \mathcal{H}$. This will be discussed in the next section.

We conclude the present section by giving the explicit expressions of the first perturbation terms, restricted to $P_o \mathcal{H}$. One finds from (4.3), (4.7) and (3.30)

$$M_{I,1}(t)\,P_0 = P_{I,1}(t)\,P_0$$

$$M_{I,2}(t)\,P_0 = \frac{1}{2}\left(P_{I,1}^2(t) + P_{I,2}(t)\right)P_0 \tag{4.19}$$

$$M_{I,3}(t)\,P_0 = \left[\frac{1}{2}\left(P_{I,1}(t)\,P_{I,2}(t) + P_{I,2}(t)\,P_{I,1}(t)\right) + P_{I,1}^3(t)\right]P_0$$

Inserting the expansions (4.8) and (4.10) in (4.6) together with (4.19) gives

$$H_{I,1}^{ef}(t)\;P_0 = P_0\,H_I(t)\,P_0$$

$$H_{I,2}^{ef}(t)\;P_0 = \frac{1}{2}\,P_0\left(H_I(t)\,P_{I,1}(t) + P_{I,1}(t)\,H_I(t)\right)P_0 \tag{4.20}$$

$$H_{I,3}^{ef}(t)\;P_0 = \frac{1}{2}\,P_0\left[\left(P_{I,1}^2(t) + P_{I,2}(t)\right)H_I(t) + H_I(t)\left(P_{I,1}^2(t) + P_{I,2}(t)\right)\right]P_0$$

In obtaining (4.20), use has been made from various identities of the type

$$P_0\,P_{I,1}(t)\;P_0 = 0\,,\quad P_0\left(P_{I,2} + P_{I,1}^2(t)\right)P_0 = 0$$

which can be deduced from (3.15).

V. COMMENTS AND EXAMPLES

We give a brief summary of the main result in the Schrödinger picture. Coming back to the Schrödinger picture amounts to perform the unitary transformation $\exp(iH_0t)$ on all the objects discussed in the previous sections. Obviously, all the norm estimates obtained in section III will remain the same.

The evolution operator (2.9) reads

$$U(t, t_0) = M(t)\;W(t, t_0)\,M^*(t_0) \tag{5.1}$$

with $M(t) = e^{-iH_0t}\,M_I(t)\,e^{iH_0t}$, $W(t, t_0) = e^{-iH_0t}\,W_I(t, t_0)\,e^{iH_0t}$.

In the Schrödinger picture, $W(t, t_0)$ obeys the equation of motion

$$i\,\frac{d}{dt}\,W(t, t_0) = H^{ef}(t)\;W(t, t_0) \tag{5.2}$$

where

$$H^{ef}(t) = H_o + \sum_{j=1}^{N} \lambda^j H_j^{ef}(t) + O(\lambda^{N+1}) \tag{5.3}$$

and $\left[H_j^{ef}(t) , P_o \right] = 0.$

As in (4.15), one will calculate with the truncated effective hamiltonian at some order $q \leq N$

$$H^{ef\,q}(t) = H_o + \sum_{j=1}^{q} \lambda^j H_j^{ef}(t) \tag{5.4}$$

and the corresponding "rotated" evolution

$$i \frac{d}{dt} W^q(t, t_o) = H^{ef\,q}(t)\ W^q(t, t_o) \tag{5.5}$$

leaves the subspaces $P_o \mathcal{H}$ and $(I-P_o)\mathcal{H}$ invariant,

$$\left[W^q(t, t_o) , P_o \right] = 0. \tag{5.6}$$

As in (4.18) and (4.19), one can calculate the full evolution in this manner

$$\begin{aligned} U(t, t_o) &= M(t)\, W^q(t, t_o)\, M^*(t_o) + O(\lambda^{q+1} |t-t_o|) \\ &= M(t)\, P_o\, W^q(t, t_o)\, P_o\, M^*(t_o) \\ &\quad + M(t)\, (I-P_o)\, W^q(t, t_o)\, (I-P_o)\, M^*(t_o) + O(\lambda^{q+1} |t-t_o|) \end{aligned} \tag{5.7}$$

The formula (5.7) is the main result of the paper : up to errors of order $O(\lambda^{q+1} |t-t_o|)$, the problem of integrating (2.8) is reduced to calculate the transformation function to some order and to integrate (5.5) separately in $P_o \mathcal{H}$ and $(I-P_o)\mathcal{H}$. If this program can be carried out, one obtains the evolution of an arbitrary initial state.

Let us mention that if

$$\int_{-\infty}^{\infty} \| H_I(t) \| \, dt < \infty \tag{5.8}$$

then all our estimations become uniform with respect to t (see e.g. Proposition 3). In particular the error term in (5.7) is $O(\lambda^{q+1})$ uniformly in t.

In its general features (although they are different at some key technical points) the theory presented above is similar to the adiabatic approximation schemes, in the sense that also in the adiabatic case the idea is to approximate the true evolution by an "adiabatic evolution" which, in an appropriately rotated frame is block diagonal (see e.g. [18-22] for the construction of various "adiabatic evolutions" and the degree they approximate the true evolution).

Let us give some simple examples.

Example 1 : non resonant two level atoms

Let $\mathcal{H}$ be two dimensional and H_0 have two non degenerate eigenvalues with eigenvectors $|n>$, n = 1, 2. Since $P_0\mathcal{H}$ and $(I-P_0)\mathcal{H}$ are one dimensional, the restriction of $W^q(t, t_0)$ to these subspaces is a simple phase factor. Then the matrix elements of $U(t, t_0)$ are given by

$$<n|U(t, t_0)|m> =$$

$$= \sum_{k=1}^{2} C_{nk}(t) \; C^{*}_{mk}(t_0) \exp\left(- i \int_{t_0}^{t} ds <k|H^{ef\,q}(s)|k> \right) + O\left(\lambda^{q+1}|t-t_0|\right) \tag{5.9}$$

with

$$C_{nk}(t) = <n|M(t)|k> \tag{5.10}$$

Example 2 : three level atom with two resonant states.

Let $\mathcal{H}$ be three dimensional, $P_0 = |1><1| + |2><2|$ the projection on the two resonant eigenstates $|1>$ and $|2>$ of H_0, and $I-P_0 = |3><3|$ be the projection on the non resonant state. Then

$$\langle n \mid U(t, t_0) \mid m \rangle = \sum_{k,\, l=1}^{2} C_{nk}(t)\, C^{*}_{m\, l}(t_0) \langle k \mid W^{q}(t, t_0) \mid l \rangle$$

$$+ C_{n\,3}(t)\; C^{*}_{m\,3}(t_0) \exp\left(- i \int_{t_0}^{t} ds \langle 3 \mid H^{ef\, q}(s) \mid 3 \rangle \right) + O\left(\lambda^{q+1} \mid t-t_0 \mid\right) \qquad (5.11)$$

where the $C_{nk}(t)$ are defined as in (5.10). In this case one still has to solve (5.5) in the two dimensional subspace of resonant states. Formula (5.11) enables to take into account the effect on the resonant dynamics of an isolated level which is energetically separated from the resonant ones.

In actual situations, $P_0\mathcal{H}$ can be finite dimensional, but $(I-P_0)\mathcal{H}$ is usually infinite dimensional (it will contain the subspace of continuous spectrum of H_0), so that the problem of integrating (5.5) in $(I-P_0)\mathcal{H}$ may turn out to be as difficult as the original one. It is therefore of interest to know what kind of information can be obtained from the mere knowledge of $W^q(t, t_0)$ restricted to $P_0\mathcal{H}$. We observe that if an initial condition ψ is chosen in the subspace $\tilde{P}(t_0)\mathcal{H}$, then by (4.2), $\psi = M(t_0)\varphi$ with φ in $P_0\mathcal{H}$. Therefore one has in this case

$$U(t, t_0)\, \psi = M(t)\, P_0\, W^{q}(t, t_0)\, P_0\, \varphi + O\left(\lambda^{q+1} \mid t-t_0 \mid\right) \qquad (5.12)$$

If by a careful adiabatic switching on one can prepare the system to be in $\tilde{P}(t_0)\mathcal{H}$ at $t = t_0$, its subsequent evolution will be determined by the knowledge of $P_0\, W^q(t, t_0)\, P_0$ and $M(t)$. However, it is more common to have the system prepared in an eigenstate of H_0 at $t = t_0$, i.e. $P_0\, \psi = \psi$. Also in this case relevant information can be obtained from (5.7) if we recall that (see (4.8))

$$M(t) = I + O(\lambda) \qquad (5.13)$$

where $O(\lambda)$ is uniform in t. Then (5.7) gives

$$U(t, t_0) = W^{q}(t, t_0) + \lambda\, O\left(1 + \lambda^{q} \mid t-t_0 \mid\right) \qquad (5.14)$$

i.e. one can compute the evolution of an initial state in $P_0\mathcal{H}$ with the help of $H^{ef\, q}(t)$ $(q \leq N)$ up to an error of order λ on time intervals of length $\mid t-t_0 \mid \approx \lambda^{-q}$.

At the first sight one may think that retaining the higher powers in λ in $P_0\, H^{ef\,q}(t)\, P_0$ is superflous in (5.14). That this is not so, one can see already in the trivial case when P_0 is one dimensional and hence

$$P_0\, W^q(t, t_0)\, P_0 = \exp\left(-i \sum_{j=0}^{q} \lambda^j e_j(t)\right) P_0$$

where

$$e_j(t) = \int_{t_0}^{t} du\ \langle 0 | H_j^{ef}(u) | 0 \rangle \quad , \qquad P_0 | 0 \rangle = | 0 \rangle \tag{5.15}$$

Now in general $\lambda^j e_j(t) = O(\lambda^j |t-t_0|)$ and becomes significant on scales $|t-t_0| = O(\lambda^{-j})$. Notice that when P_0 is not one dimensional the phases in $P_0\, W^q(t,t_0)\, P_0$ enter the expressions of the resonant transitions, so (5.14) implies that the necessary and sufficient condition for $P_0\, W^q(t,t_0)\, P_0$ to describe all resonant effects on scales $|t-t_0| \leq \lambda^{-q}$ is to retain the first q terms in the expression of $P_0\, H^{eff}\, P_0$.

The main result of the section 3 was that one can construct initial conditions $\tilde{P}(t_0)$ such that P(t) (see (2.19)) has on expansison in λ up to the "resonant"order with uniformly bounded coefficients. One can see that in general this is not the case for arbitrary initial conditions. For shortness let us illustrate the matter on the simple case in example 1. Let $|n(t_0)\rangle = M(t_0)|n\rangle$ and ψ an arbitrary state. If we write

$$\psi = \sum_{n=1}^{2} a_n |n(t_0)\rangle = M(t_0) \sum_{n=1}^{2} a_n |n\rangle$$

then

$$P(t) = U(t, t_0)\, |\psi\rangle\langle\psi|\, U^*(t, t_0) =$$

$$\sum_{n,m=1}^{2} a_n a_m^* \exp\left(-i \int_{t_0}^{t} ds\, \Delta_{n,m}^{N}(s)\right) M(t)\, |n\rangle\langle m|\, M^*(t) + O\left(\lambda^{N+1} |t-t_0|\right)$$

where (5.16)

$$\Delta_{n,m}^{N}(t) = \langle n | H^{ef\,N}(t) | n\rangle - \langle m | H^{ef\,N}(t) | m\rangle \tag{5.17}$$

In general for $n \neq m$ $\Delta^N_{n,m}(t)$ do not have expansions in λ with uniformly bounded coefficients, and then the same is true for P(t). Of course if one of the a_n equals zero we are back to the "good" initial conditions. Let us stress however that if the hamiltonian involved is such that $\Delta^N_{n,m}(t)$ do not depend on λ, then of course "nice" expansions exist for arbitrary initial conditions.

We shall end by illustrating on a solvable example (the driven harmonic oscillator) that actually stronger results can be obtained in specific cases. We consider an harmonic oscillator $H_o = \omega\, a^*a$ of frequency ω submitted to the external time-dependent potential $\lambda f(t)\,(a + a^*)$, and denote $|n>$, $n = 0, 1, 2 \ldots$ the eigenstates of H_o, with eigenvalues $n\omega$. If the projection $|0><0|$ on the ground state is chosen as initial state at time t_o, it is well known that its time evolution is given by [23]

$$U_I(t, t_o)\,|0><0|\,U_I^*(t, t_o) = |\alpha(t, t_o)><\alpha(t, t_o)| \tag{5.18}$$

where $|\alpha(t, t_o)>$ is a coherent state represented in the $\{|n>\}$ basis by

$$|\alpha(t, t_o)> = \exp\left(-\frac{1}{2}\lambda^2\,|\alpha(t, t_o)|^2\right)\sum_{n=0}^{\infty}\frac{(\lambda\alpha\,(t, t_o))^n}{\sqrt{n\,!}}\,|n> \tag{5.19}$$

$$\alpha(t, t_o) = -i\int_{t_o}^{t} ds\, e^{i\omega s}\, f(s) \tag{5.20}$$

In the case of adiabatic switching on, the time evolved projection $P_I^{\varepsilon}(t)$ is given by the same formulae (5.18) and (5.19) with $\alpha(t, t_o)$ replaced by

$$\alpha^{\varepsilon}(t) = -i\int_{-\infty}^{t} ds\, e^{i(\omega - i\varepsilon)s}\, f(s) \tag{5.21}$$

Hence

$$P_I^{\varepsilon}(t) = \exp\left(-\lambda^2\,|\alpha^{\varepsilon}(t)|^2\right)\sum_{n,m=0}^{\infty}\frac{(\lambda\,\alpha^{\varepsilon}(t))^n}{\sqrt{n!}}\,\frac{(\lambda\,\alpha^{\varepsilon}(t))^m}{\sqrt{m!}}\,|n><m| \tag{5.22}$$

Since the operators $|n\rangle\langle m|$ have a norm equal to one, these series are norm convergent for any value fo λ.

Consider now the following two cases

a) $f(t) = \cos \omega_0 t \ , \ \omega_0 \neq \omega$

so that

$$\lim_{\varepsilon \to 0} \alpha^{\varepsilon}(t) = \alpha(t) = e^{i\omega t} \left(\frac{\omega \cos \omega_0 t - i \omega_0 \sin \omega_0 t}{\omega_0^2 - \omega^2} \right) \tag{5.23}$$

b) $\int_{-\infty}^{\infty} dt\, |f(t)| < \infty$ $\qquad$ ($\hat{f}(\omega)$ is continuous)

so that

$$\lim_{\varepsilon \to 0} \alpha^{\varepsilon}(t) = \alpha(t) = -i \int_{-\infty}^{t} ds\, e^{i\omega s} f(s) \tag{5.24}$$

We conclude in both cases from (5.23) and (5.24) that the series (5.22) have a term by term limit as $\varepsilon \to 0$, and

$$\text{n-}\lim_{\varepsilon \to 0} P_I^{\varepsilon}(t) = P_I(t) = P_0 + \sum_{k=1}^{\infty} \lambda^k P_{I,k}(t) \tag{5.25}$$

The norm convergent perturbation series (5.25) can be obtained explicitely from (5.22) with $\alpha^{\varepsilon}(t)$ replaced by $\alpha(t)$, and reorganizing the powers of λ.

Applying the proposition 2 to the case (a) with $\omega_0 = \omega/2$ we would only conclude that $P_{I,1}^{\varepsilon}(t)$ has a limit, since already at the order 2 a resonance could in principle occur with the eigenvalue 2ω of H_0. Nevertheless $P_I(t)$ has a full perturbation expansion because of the peculiar properties of the oscillator and of the interaction (equidistant levels and V(t) connects only the state $|n\rangle$ to $|n \pm 1\rangle$). In the case (b), assuming for instance that the support of $\hat{f}(\omega)$ is the entire real line, we could not draw any informative conclusion from proposition 2. The fact that $P_I(t)$ has complete perturbation series is due here to the smoothness of $\hat{f}(\omega)$ (but the $P_{I,n}(t)$ are no more given by the formula (3.14)).

Acknowledgements

G. N. would like to thank the Institute of Theoretical Physics - EPF-Lausanne for hospitality and financial support during this work.

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