THEORETICAL CHEMISTRY INSTITUTE

THE UNIVERSITY OF WISCONSIN

TIME-DEPENDENT PERTURBATION OF A TWO-STATE QUANTUM MECHANICAL SYSTEM

David Roger Dion

WIS-TCI-502

7 June 1974

(NASA-CR-139250) TIME-DEPENDENT PERTURBATION OF A TWO-STATE QUANTUM MECHANICAL SYSTEM (Wisconsin Univ.) 341 p HC $20.25 CSCL 12A

N74-30028

Unclas
G3/19 54893

MADISON, WISCONSIN

TIME-DEPENDENT PERIODIC PERTURBATION OF A TWO-LEVEL QUANTUM SYSTEM*

David Roger Dion

(Under the supervision of Professor Joseph O. Hirschfelder)

ABSTRACT

This thesis is concerned with a two- (non-degenerate) level quantum system interacting with a classical monochromatic radiation field.

The existing work on this problem is reviewed and some novel aspects of the problems are presented. The new contributions are:

(1) The problem is treated in a more general manner than previously: all values of the four essential parameters are considered; a diagram shows which of thirteen methods is optimum for a given parameter range; each of these methods is derived and discussed; and, three of these methods (T3, T5 and T8) are novel.

(2) Using the Floquet (1883)-Poincaré (1892,1893,1899) theory and following Shirley (1963,1965), the time-dependent parts of the

* Supported by the National Aeronautics and Space Administration Grant NGL-50-002-001 and the National Science Foundation Grant GP-28213.

wavefunction are Fourier analyzed to obtain an equation analogous to a static "Schrödinger Equation." The Fourier Expansion Coefficients play the role of an orthonormal complete basis. The Floquet characteristic exponent, μ , plays the role of energy. Zeroth-order exact degeneracies occur when the time-dependent perturbation is weak and its angular frequency is very large. Here, standard degenerate Rayleigh-Schrödinger perturbation theory is used to give novel solutions (T5).

(3) Resonances correspond to zeroth-order almost degeneracies in the static problem. Certain-Hirschfelder (1970a,b,c) partitioning perturbation theory (T6 and T7) is used to overcome difficulties inherent in using Salwen's (1955) (used by Shirley) or Winter's (1959) almost degenerate perturbation theories.

(4) When no near or exact zeroth-order degeneracies occur in the static problem, non-degenerate Rayleigh-Schrödinger perturbation theory is used to obtain T1-solutions. It is shown that these solutions are equivalent to Sen-Gupta's (1970) solutions (T2).

(5) The Langhoff-Epstein-Karplus (1972) factorization of the time-dependent wavefunction is applied to the two-level system and, novel approximations, (T3), to the two Floquet Solutions are thereby obtained.

(6) Solutions for the two-level system are obtained by using the Langhoff-Epstein-Karplus (1972) formalism (which was formulated

for the infinite-level system). The adiabatic turn-on is <u>explicitly</u> considered and the following important properties of the resulting solutions are emphasized:

(a) The solutions are of the Floquet form: $\Phi(\underset{\sim}{r},t)\ \exp[-i\mu\tau]$; where Φ is a space-dependent function periodic in the time, and μ is a constant.

(b) The solutions illustrate Young and Deal's (1970) adiabatic theorem which asserts that an adiabatic turn-on of a periodic perturbation puts a system in a Floquet Mode Solution.

(c) The solutions converge asymptotically whenever the energy splitting divided by angular frequency almost equals a non-zero positive integer because of almost vanishing denominators. The Langhoff-Epstein-Karplus solutions for the infinite-level system near resonances should have the same sort of asymptotic convergence difficulties.

(7) If $a(\tau)$ and $b(\tau)$ are the wavefunction's time-dependent coefficients, then, the equations for $(a(\tau)/b(\tau))$ and $(b(\tau)/a(\tau))$ are treated by singular perturbation theory (T8) to obtain the two Floquet Solutions for $a(\tau)$ and $b(\tau)$ as power series expansions in powers of the angular frequency divided by the energy splitting. This novel treatment is peculiar, since, the singular perturbation solutions

(a) do not, in general, behave like outer solutions.

(b) may be used to generate both linearly independent Floquet Solutions without ever having to find "inner solutions."

(8) The Floquet-Poincaré Theory allows $a(\tau)$ and $b(\tau)$ to be of the form $\tau\phi(\tau)\exp[-i\mu\tau]$ where ϕ is periodic and μ is constant. Whereas previous authors have not even considered this, in Chapter III a proof that it cannot occur is given.

To my parents, Ann and Ernest Dion

ACKNOWLEDGEMENTS

It is a pleasure to express my thanks to the following people without whose help this thesis would not exist:

Professor J. O. Hirschfelder for his guidance of my graduate research, for his encouragement in times of discouragement, for his efforts in providing the excellent resources and atmosphere of the Theoretical Chemistry Institute, and finally, for his friendship.

Professors L. W. Bruch, P. R. Certain, C. F. Curtiss, S. T. Epstein, and J. E. Harriman for their constant willingness to help.

Ms. Patty Spires for her excellent job in typing this thesis.

Mrs. Gloria Lawton and Mr. Jerry Carrig for seemingly countless instances of help.

The taxpayers of Wisconsin for maintaining the University of Wisconsin.

The taxpayers of the United States for funding this work through the National Science Foundation and the National Aeronautics and Space Administration.

My friends, for their friendship.

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INTRODUCTION

Motivation

The Semi-Classical Theory of the interaction of radiation and matter combines the great triumph of Nineteenth Century physics, Maxwell's Equations, with the great triumph of Twentieth Century Physics, the laws of quantum mechanics. In the Semi-Classical Theory, the electromagnetic radiation is described by Maxwell's Equations, and, the radiation field is thereby specified with arbitrary accuracy. The material system, however, is described by the laws of quantum mechanics.

Although, as Dirac (1927) first showed, the field may also be quantized, the Semi-Classical Theory alone explains many phenomena. Wentzel (1927) described the photoelectric effect, Klein and Nishina (1929) correctly explained the scattering of radiation from a free electron and Klein (1927) treated absorption and stimulated emission of radiation by an atom, without quantizing the field. Bloembergen (1965) has treated nonlinear optics in a completely Semi-Classical manner. In fact, it is generally conceded that the radiation field needs to be quantized only in treating such phenomena as the Lamb Shift and the Spontaneous Emission of radiation.

In this thesis we are concerned with the simplest Semi-Classical system: one in which the quantum system has only two energy levels and the classical radiation field is monochromatic. In spite of its simplicity, it is an important system. A thorough understanding of it is a necessary prelude to the thorough understanding of a many-leveled quantum system in a classical field. It is an interesting system since it exactly corresponds to a spin ½ particle in a sinusoidally oscillating electric or magnetic field. It is also a good model for a many-leveled system in which only two states strongly interact under the influence of the time-varying field.

The two-level system is Semi-Classically described by two first order, coupled, linear, homogeneous differential equations with periodic coefficients. Floquet (1883) studied the solutions of the general n-th order linear differential equation with periodic coefficients and Poincaré (1892,1893,1899) investigated the practical construction of such solutions. Moulton (1920,1930) completely describes the solutions for n first order coupled, linear, homogeneous differential equations with periodic coefficients. From these studies, the functional form of the solution to the two-level system is known. In spite of this fact, a closed form solution has never been found. Many authors have sought approximate solutions and their studies appear under such diverse titles as "Stark Effect in Rapidly Varying Fields"* and "Optical Pumping and Related Topics."† Furthermore, the appropriate approximate technique depends on the

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* Autler and Townes (1955).

† Series (1970).

field's strength, its frequency and the magnitude of the energy splitting.

No review of the two-level problem appears in the literature, and, there is therefore a need for a systematic, complete review of the problem. This thesis is an attempt to fill that need. However, this thesis is more than a review since it discusses some novel aspects of the problem. These new contributions are:

(1) Treating the problem in a more general fashion than previous authors:

(a) If $\psi_a(\underset{\sim}{r})$ and $\psi_b(\underset{\sim}{r})$ are the wavefunctions for the two states and $V(\underset{\sim}{r})$ is the spatial part of the time-dependent perturbation, then most authors consider $V_{ab} = \langle\psi_a(\underset{\sim}{r})|(V(\underset{\sim}{r})|\psi_b(\underset{\sim}{r})\rangle$ but neglect V_{aa} and V_{bb}. We consider V_{aa} and V_{bb} as well as V_{ab}.

(b) We introduce into the Hamiltonian, an operator $\hat{\gamma}$ which allows for transitions out of either of the two levels which are not caused by the time-dependent perturbation. However, $\hat{\gamma}$ does not allow for spontaneous transitions from the upper to the lower state.

(c) <u>All possible values</u> of the four essential parameters occurring in the problem are considered.

(d) A diagram, Figures VI-A and VI-B, is given which shows which technique is best to use for any particular choice of parameters. There are eight different perturbation methods and three numerical techniques which are optimum for different ranges of the parameters. This diagram summarizes our study of the convergence and range of applicability of a total of nine perturbation techniques and four numerical techniques.

(2) Using the Floquet (1883)-Poincaré (1892, 1893, 1899) Theory, we follow Shirley (1963,1965) and Fourier analyze the time-dependent parts of the wavefunction to obtain an equation analogous to a static "Schrödinger Equation." The Fourier Expansion Coefficients play the role of an orthonormal basis set which spans the space of the "time-independent Hamiltonian." The Floquet characteristic exponent, μ , plays the role of energy. When the angular frequency of the time-dependent perturbation is much larger than any of the system's resonance frequencies, there is a zeroth-order double degeneracy between each of the Fourier components of state a and the corresponding Fourier component of state b . Our new contribution is to solve the problem of the perturbation's effect by using standard degenerate Rayleigh-Schrödinger Perturbation Theory. This new method is T5.

(3) Resonances occur whenever the ratio of the energy splitting to the perturbation's angular frequency is almost equal to a positive non-zero integer, n . In the static formulation, this corresponds to a zeroth-order almost degeneracy between the j-th Fourier Component of state a and the (j-n)-th Fourier Component of state b . This correspondence has been noted before by Winter (1959) and Shirley (1963,1965). Our contribution is

(a) using the Certain-Hirschfelder (1970a, b, c) partitioning perturbation theory to handle these resonant almost-degeneracies (T6, T7).

(b) demonstrating that Certain-Hirschfelder theory is the preferred way to treat these almost degeneracies.

Shirley treated them by using Salwen's (1955) almost degenerate perturbation theory which, as we prove in Chapter XI, will not yield exact results even if carried to infinite order. Winter's scheme (which is Heitler's (1960) perturbation theory extended to handle almost degeneracies) cannot be used to treat the non-hermitian static Hamiltonian which arises when the rate of non-radiative transitions out of state a does not equal the rate of non-radiative transitions out of state b . We use "non-radiative transitions" to mean those transitions not caused by the time-dependent perturbation (i.e. those caused by the introduction of the operator $\hat{\gamma}$ into the Hamiltonian).

(4) We take note of the fact that when the time-dependent perturbation's angular frequency is less than the highest resonant frequency but not almost equal to any of the resonance frequencies or zero, then no Fourier Coefficients are almost or exactly degenerate. Here, standard non-degenerate Rayleigh-Schrödinger perturbation theory is used to obtain approximate solutions (T1) which are equivalent to the solutions obtained by application of Sen Gupta's (1970) technique (T2). Our contribution here is to show that even though T2 does not involve a reduction of the original time-dependent problem to a static problem, it is equivalent to doing so and then using standard non-degenerate Rayleigh-Schrödinger Perturbation Theory.

(5) Langhoff, Epstein, and Karplus (1972) develop a formalism for finding the steady-state solutions for the general quantum

system, i.e., the solutions which arise when the quantum system is in one of its non-degenerate stationary states before the time-dependent periodic perturbation is adiabatically turned-on. An aspect of their treatment is writing the time-dependent wavefunction as a time- and space-dependent periodic part multiplying an exponentiated part. The argument of the exponent only depends on time and it consists of terms linear in time and terms periodic in time. Our minor contribution here is the simple application of their factorization to the two-level system to obtain novel approximate solutions (T3) to the two linearly independent Floquet Solutions.

(6) The Langhoff, Epstein, and Karplus (1972) paper gives a method of finding the steady-state solutions for a general quantum system. Their formalism is applied to the two-level system and solutions are thereby obtained. The adiabatic turn-on is explicitly considered and the following points about the two-level solutions are emphasized:

(a) The solutions are of the Floquet form: $\Phi(\underset{\sim}{r},t)\exp[-i\mu\tau]$; where Φ depends on spatial coordinates and is periodic in the time, and μ is constant.

(b) The solutions illustrate Young and Deal's (1970) assertion that turning a periodic perturbation on adiabatically brings the system into a Floquet Normal Mode Solution.

(c) The solutions converge asymptotically whenever the ratio of the energy splitting to the perturbation's angular frequency is almost equal to a positive non-zero integer because of almost vanishing denominators. The same convergence difficulties should occur when the Langhoff-Epstein-Karplus technique is applied to the infinite-level system near a resonance.

We have privately communicated the foregoing convergence analysis to S. Epstein and P. Langhoff and they said they were aware of these difficulties. No such analysis, however, appears in the literature and we therefore feel that putting this discussion of convergence in print is a contribution.

(7) Another novel contribution is the use of singular perturbation theory, in Chapter XIII, to find linearly independent Floquet Solutions as a power series expansion in $(1/\varepsilon)$, where, ε is the energy splitting divided by the angular frequency. These solutions converge in a range of parameters not covered by any previous perturbation treatments: the regime in which both the field strength and energy splitting are large compared to the angular frequency of the time-dependent perturbation. Singular perturbation theory is used to find outer solutions for $(a(\tau)/b(\tau))$ and $(b(\tau)/a(\tau))$ where $a(\tau)$ and $b(\tau)$ are the time-dependent coefficients of $\psi_a(\underset{\sim}{r})$ and $\psi_b(\underset{\sim}{r})$. The Floquet Solutions for $a(\tau)$ and $b(\tau)$ are then recovered from these quotients. A unique feature of this treatment is that inner solutions are never needed: the outer solution for $(a(\tau)/b(\tau))$ is the inner solution for $(b(\tau)/a(\tau))$ and <u>vice-versa</u>. We have not found any other example of singular perturbations having this unique feature.

(8) We prove that general solutions for $a(\tau)$ and $b(\tau)$ which contain terms of the form

$$\tau\phi(\tau)e^{-i\mu\tau}$$

(where μ is a constant and $\phi(\tau)$ is a periodic function), may never occur. (See Chapter III.)

Summary

The two-level system's Semi-Classical Hamiltonian is written down in Chapter I. None of the spatial-interaction-operator's matrix elements are allowed to vanish and we phenomenologically allow for non-radiative transitions out of either of the two levels by the introduction of an operator $\hat{\gamma}$. ($\hat{\gamma}$ does not, however, take into account spontaneous transitions from the upper to the lower of the two states.)

The Dirac form of solution is assumed:

$$\Psi(\underset{\sim}{r},t) = \eta_a(t)\psi_a(\underset{\sim}{r}) + \eta_b(t)\psi_b(\underset{\sim}{r})$$

where the two states are labelled "a" and "b". From the Schrödinger Equation, we derive differential equations for η_a and η_b.

In Chapter II, a new independent variable, τ, is introduced and new functions $a(\tau)$ and $b(\tau)$ are defined in terms of η_a and η_b. Eqs. (II-4) and (II-5) are taken as the working equations for the entire thesis since they contain only four independent parameters, whereas, the equations for η_a and η_b contain eight independent parameters. The four independent parameters are called α, β, ε and δ. α and β are related to the field strength and the magnitude of the spatial-interation-operator's matrix elements. ε is related to the energy separation between levels and δ is related to the rate of non-radiative transition out of either of the two levels.

In Chapter III, we describe the three possible functional forms of the exact general solution. Proofs of these are given in Appendix A. The general solutions are arbitrary linear combinations of two normal (or Floquet) modes. These Floquet modes involve a characteristic constant (or exponent), μ, and periodic functions, ϕ, which have the same periodicity as the $\cos\tau$-perturbation. One of the three possible forms (Form III: see Eq. (III-12)) contains terms linear in τ. We give a proof that solutions of this form cannot occur for the two-level system, whereas, previous authors have not even considered the possibility of Form III solutions. Chapter III also includes derivations of some useful properties of the exact solutions.

There are four limits in which exact solutions to Eqs. (II-4) and (II-5) are known. These are discussed in Chapter IV. We find, however, that no one perturbation technique solves the problem for arbitrary values of α, β, δ and ε. In fact, nine different perturbation techniques (Techniques T1 through T9) are described in this thesis. For some values of α, β, δ and ε, no perturbation solutions have been found and numerical techniques must be used.

Four such numerical techniques are given and they are Techniques T10 through T13.

The thirteen techniques are listed in Table VI in Chapter VI. This table gives the descriptive name of each technique, its range of applicability and where, in this thesis, it is discussed. Figures (VI-A) and (VI-B) diagrammatically indicate which technique is best depending on the values of α, β, δ and ϵ. Throughout this thesis, care has been taken to note the range of convergence of each and every perturbation technique. Not all of the thirteen techniques are totally distinct. Techniques T1 and T2 are, respectively, just the static and dynamic formulation of the same approximation scheme. Techniques T3 and T4 are equivalent if δ vanishes. T6 and T7 are essentially identical and we split them up for organizational purposes.

Following Shirley (1963,1965), the dynamic problem of Eqs. (II-4) and (II-5) is transformed into a static eigenvalue-eigenvector problem in Chapter V. With this transformation, the whole arsenal of quantum mechanical stationary state approximation techniques can be brought into play. For example, non-degenerate Rayleigh-Schrödinger Perturbation Theory (its formulation and convergence is discussed in Chapter VII) is used as Technique T1. It is shown to be the static equivalent of Sen Gupta's (1970) treatment which is called T2.

In Chapter VIII we also describe T3: solving the equations for the quotients $a(\tau)/b(\tau)$ and $b(\tau)/a(\tau)$ by a perturbation expansion in the field strength. Although no other authors have specifically treated the two-level problem in this manner, T3 is merely an application of a more general time-dependent perturbation theory given by Langhoff, Epstein, and Karplus (1972). T4 is the Langhoff-Epstein-Karplus (1972) "steady-state" perturbation theory and we hopefully clarify their formalism by applying it to the two-level system with $\delta = 0$.

T5 is the application of degenerate Rayleigh-Schrödinger perturbation theory to the static eigenvalue-eigenvector problem. This technique, which is described in Chapter IX, yields novel approximations to the problem.

When the radiation's angular frequency, ω , is such that $\hbar n\omega \approx \Delta W$ (where ΔW is the energy difference between states and n is a positive non-zero integer), zeroth order near (or exact) degeneracies occur in the static formulation of the problem. This difficulty is overcome by using the Certain-Hirschfelder (1970a,b,c) partitioning perturbation theory which is described and discussed in Chapter X.

The case of $\hbar\omega = \Delta W$ corresponds to the main resonance. In Chapter XI, the Certain-Hirschfelder theory is applied to this case (T6). We also discuss the treatments of the two-level system's main resonance given by Rabi (1937), Bloch and Siegert (1940), Stevenson (1940), Shirley (1963,1965), Silverman and Pipkin (1972), Winter (1959) and Pegg (1973b). Where appropriate, these techniques are compared to T6. Shirley's formulation of the main resonance differs from ours only in the perturbation theory used: he uses a perturbation theory due to Salwen (1955). At the conclusion of

Chapter XI we therefore show how Salwen's perturbation theory will not give exact results even if it is carried to infinite order.

Technique T7 is introduced in Chapter XII and it is just the Certain-Hirschfelder partitioning perturbation theory applied to the sub-harmonic resonances where sub-harmonic resonances occur whenever $\hbar n_r \omega \simeq \Delta W$ (n_r is a integer greater than unity). We find that depending on the values of n_r, β and N (where N is the order of field strength through which the solutions are correct), T7 is equivalent to T1. We, therefore, give Figure (XII-A) which diagrammatically tells when T1 is preferred over T7. Chapter XII concludes with a discussion of Shirley's (1963,1965), Pegg's (1973b) and Winter's (1959) work. Particular attention is paid to Winter's (1959) treatment, because, although his formulation is quite different from T7, we show that his results are exactly the T7 results when $\delta = 0$ and "Certain-full-normalization" is used in T7.

Chapter XIII contains the most novel aspect of this thesis: the application of singular perturbation theory to the two-level system (T8). In Technique T8 we solve the equation for $b(\tau)/a(\tau)$ to find one Floquet Mode as a power series in inverse powers of ε. We then solve the equation for $a(\tau)/b(\tau)$ to find the other Floquet Mode as a power series in inverse powers of ε. Even though singular perturbation theory is utilized to obtain both solutions, we obtain the anomolous result that

(a) the singular perturbation solutions do not, in general, behave like outer solutions.

(b) the singular perturbation solutions may be used to generate both linearly independent Floquet solutions. Thus, we never need to find "inner solutions."

The final perturbation technique, T9, is introduced in Chapter XIV. T9 has been used by Shirley (1963) and Series (1970) and it is extended to include non-vanishing values of the parameters β and δ. This technique is useful when the applied field is quite strong compared to the energy splitting between states. It is formulated as a matrix eigenvalue-eigenvector problem which is solved by degenerate Rayleigh-Schrödinger Perturbation Theory.

The main body of this thesis concludes with four numerical techniques which are to be used when α, β, δ and ε are such that no perturbation techniques are available. These numerical techniques are introduced and compared in Chapter XV.

Chapter XVI contains a recipe for using the Meadows (1962)-Ashby (1968) numerical technique (T10). It consists of finding the characteristic exponent, μ, by solving a transcendental equation for μ which involves the determinant of a μ-independent infinite matrix. The exact form of the transcendental equation depends on whether δ vanishes and whether ε is almost (or exactly) equal to an even integer. We therefore distinguish between Case A (Eq. (XVI-2)) and Case B (Eq. (XVI-4)). These two equations are derived and the chapter concludes with a discussion of numerically finding the Fourier Expansion Coefficients of the Floquet "ϕ-functions."

T11 (the Autler-Townes (1955) numerical solution) is described and derived in Chapter XVII. It consists of finding μ by numerically solving Eq. (XVII-1) which is an equation equating μ with the sum of two infinite continued fractions which themselves contain μ. The Fourier Expansion Coefficients are found by evaluating μ-dependent infinite continued fractions. β must vanish if T11 is to be used.

T12 is introduced in Chapter XVIII. It is simply direct computer diagonalization of a real, symmetric tridiagonal matrix. It only applies when <u>both</u> δ and β vanish.

The last numerical technique (T13) applies for arbitrary values of α, β, δ and ε. It is discussed in Chapter XIX and it involves direct numerical solution of Eqs. (II-4) and (II-5) for specified initial conditions. These solutions are used to construct a 2×2 matrix, the eigenvalues of which are directly related to the characteristic exponents (see Eq. (XIX-12)).

There are two appendices. Appendix A contains an exposition of Floquet Theory and Appendix B contains a discussion of the equations for $a^*(\tau)a(\tau)$, $b^*(\tau)b(\tau)$ and $a^*(\tau)b(\tau)$. References are placed after the appendices.

I. FORMULATION OF THE PROBLEM

The Hamiltonian for the two-level system is given by (I-1).

$$H = H^0(\underset{\sim}{r}) + 2FV(\underset{\sim}{r})\cos\omega t - i\frac{\hat{\gamma}}{2} \qquad \text{(I-1)}$$

In (I-1) $\hbar$ has been set equal to unity, $H^0(\underset{\sim}{r})$ is the Hamiltonian for the unperturbed system for which

$$H^0(\underset{\sim}{r})\psi_j(\underset{\sim}{r}) = W_j\psi_j(\underset{\sim}{r}) \qquad j=a,b\ .$$

For convenience we will define $W_b > W_a$. F is the field strength and the field interacts with the system through the interaction operator $V(\underset{\sim}{r})$. The operator $\hat{\gamma}$ is defined by:

$$\hat{\gamma}\psi_a(\underset{\sim}{r}) = \gamma_a\psi_a(\underset{\sim}{r}) \quad \text{and} \quad \hat{\gamma}\psi_b(\underset{\sim}{r}) = \gamma_b\psi_b(\underset{\sim}{r})$$

γ_a and γ_b are scalars. The effect of $\hat{\gamma}$ is to introduce damping constants into the wavefunctions. Thus, $\hat{\gamma}$ takes into account in a phenomenological way transitions away from levels ψ_a and ψ_b which we are not explicitly considering (Weisskopf (1930). Also see Maitland (1969), Chap. 3, Sec. 3)). These "away transitions" could be, for instance, spontaneous relaxation by emission of radiation, collisional de-excitation, or relaxation by giving up energy which goes into lattice excitation. Whatever the "away transitions" are, they can be taken into account by the inclusions of $\hat{\gamma}$ as long as these transitions obey a linear rate law.

If γ_a and γ_b are not <u>both</u> zero, the normalization of the wavefunction for the two state system is not preserved. Note that this present formulation, with $\hat{\gamma}$ defined the particular way it has been defined, does not take into account spontaneous transitions from the upper to the lower of the two states.

The time dependent Schrödinger equation for the system is:

$$i\dot{\Psi}(\underset{\sim}{r},t) = H\Psi(\underset{\sim}{r},t) \qquad \text{(I-2)}$$

In (I-2), $\hbar$ has again been set equal to unity and the dot over Ψ denotes differentiation with respect to time. Assuming that

$$\Psi(\underset{\sim}{r},t) = \eta_a(t)\psi_a(\underset{\sim}{r}) + \eta_b(t)\psi_b(\underset{\sim}{r}) \qquad \text{(I-3)}$$

substitution of (I-3) into (I-2) yields equations for η_a and η_b

$$i\dot{\eta}_a = W_a\eta_a - i\,\frac{\gamma_a}{2}\,\eta_a + 2FV_{aa}\cos\omega t\eta_a + 2FV_{ab}\cos\omega t\eta_b \qquad \text{(I-4)}$$

$$i\dot{\eta}_b = W_b\eta_b - i\,\frac{\gamma_b}{2}\,\eta_b + 2FV_{ab}\cos\omega t\eta_a + 2FV_{bb}\cos\omega t\eta_b \qquad \text{(I-5)}$$

$$V_{ij} \equiv \langle\psi_i(\underset{\sim}{r})|V(\underset{\sim}{r})|\psi_j(\underset{\sim}{r})\rangle$$

(I-4) and (I-5) are the time-dependent equations about which we will be concerned in the rest of this report.

II. STATEMENT OF WORKING EQUATIONS

The time-dependent equations (I-4) and (I-5) can be simplified by replacing $\eta_a(t)$ and $\eta_b(t)$ by the new variables $a(t)$ and $b(t)$ which are defined by

$$\eta_a(t) = a(t)\exp[-iW_a t - \frac{\gamma_a}{2} t - 2i \frac{FV_{aa}}{\omega} \sin \omega t] \qquad \text{(II-1)}$$

$$\eta_b(t) = b(t)\exp[-iW_a t - \frac{\gamma_a}{2} t - 2i \frac{FV_{aa}}{\omega} \sin \omega t] \qquad \text{(II-2)}$$

Then if we let $\omega t = \tau$ and define the following reduced parameters:

$$\varepsilon = (W_b - W_a)/\omega \quad , \quad \alpha = FV_{ab}/\omega$$
$$\beta = F(V_{bb} - V_{aa})/\omega \quad , \quad \delta = \tfrac{1}{2}(\gamma_b - \gamma_a)/\omega \qquad \text{(II-3)}$$

equations (I-4) and (I-5) become,

$$\dot{a}(\tau) = -2i\alpha(\cos\tau)b(\tau) \qquad \text{(II-4)}$$

$$\dot{b}(\tau) = -i(\varepsilon - i\delta + 2\beta\cos\tau)b(\tau) - 2i\alpha(\cos\tau)a(\tau) \qquad \text{(II-5)}$$

We will take equations (II-4) and (II-5) to be the working equations for the rest of this report. They are convenient since they only involve four independent parameters whereas equations (I-4) and (I-5) had eight independent parameters.

In Appendix B, the time-dependent equations are expressed in terms of the square of the amplitudes $a^*(\tau)a(\tau)$ and $b^*(\tau)b(\tau)$ as well as the correlation function $a^*(\tau)b(\tau)$. However, these equations are not used in the remainder of this report since they offer no advantages in terms of simplifying the mathematics. For the case of $\delta = 0$, these amplitude equations are, however, analogous to certain classical vector equations (Feynman (1957)) and they therefore enable us to relate the two-level time-dependent problem to the easily visualized problem of a constant-length three-dimensional vector rotating in space.

III. THE EXACT SOLUTION

Although we are ignorant of the exact solution of equations (II-4) and (II-5) in terms of elementary functions, we know its exact functional form from the Poincaré-Floquet* theory which is explained in detail in Appendix A. The Poincaré-Floquet treatment is used in many branches of applied mathematics. In the present section some of the theorems are given and specific applications to the present problem are pointed out.

To fit equations (II-4) and (II-5) into the notation used in Appendix A, let

$$x_1 = a(\tau) \ , \quad x_2 = b(\tau)$$

If there are two sets of particular solutions $\{a_1(\tau), b_1(\tau)\}$ and $\{a_2(\tau), b_2(\tau)\}$, then, in the notation of Appendix A, $a_1(\tau) = x_{11}$, $b_1(\tau) = x_{21}$ and $a_2(\tau) = x_{12}$ and $b_2(\tau) = x_{22}$.

If we further let

$$\theta_{11}(\tau) = 0 \qquad \theta_{12}(\tau) = -2i\alpha\cos\tau$$

$$\theta_{21}(\tau) = -2i\alpha\cos\tau \quad \theta_{22}(\tau) = -i(\varepsilon - i\delta + 2\beta\cos\tau)$$

---

* Moulton (1930), Chap. XVI. For less detailed discussions see: Ince(1956), Sect. 15.7.; Margenau (1956), pg. 80. Brillouin (1948 and 1950) also discusses the Poincaré-Floquet theory.

Then equations (II-4) and (II-5) become a special case of the following set of homogeneous linear differential equations.

$$\frac{dx_1(\tau)}{d\tau} = \theta_{11}(\tau)x_1(\tau) + \theta_{12}(\tau)x_2(\tau)$$

$$\frac{dx_2(\tau)}{d\tau} = \theta_{21}(\tau)x_1(\tau) + \theta_{22}(\tau)x_2(\tau) \qquad \text{(III-1)}$$

Floquet-Poincaré Theory for Periodic Equations

If, in (III-1), the time-dependent functions, θ_{ij} , are periodic with the period of 2π ,

$$\theta_{ij}(\tau + 2\pi) = \theta_{ij}(\tau) , \qquad \text{(III-2)}$$

then the solutions to (III-1) are arbitrary linear combinations of two normal modes. The normal (or Floquet) modes involve a characteristic constant (or exponent), μ , and functions, ϕ . The ϕ's have the same periodicity as the θ_{ij}'s . Thus

$$\phi(\tau + 2\pi) = \phi(\tau) . \qquad \text{(III-3)}$$

(n.b., these are not to be confused with the "capped" $\hat{\phi}$'s in Appendix A.) There are only three possible forms* which the solution can take.

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* It should be noted that most statements of Floquet's theorem which appear in the literature are incomplete, i.e. they only allow for "Form I". Moulton (1930), however, gives a very complete statement and our discussion, in Appendix A, is complete for the two-level system.

Form I. $(\mu_1 \neq \mu_2 + n$, n any integer or zero)

The two modes are

$$\{x_1 = e^{-i\mu_1\tau}\phi_{11} , \quad x_2 = e^{-i\mu_1\tau}\phi_{21}\} \tag{III-4}$$

and

$$\{x_1 = e^{-i\mu_2\tau}\phi_{12} , \quad x_2 = e^{-i\mu_2\tau}\phi_{22}\} \tag{III-5}$$

These linearly independent solutions may be linearly combined to form a general solution given by (III-6). The constants C_1 and C_2 are chosen to satisfy initial conditions.

$$\begin{aligned} x_1 &= C_1 e^{-i\mu_1\tau}\phi_{11} + C_2 e^{-i\mu_2\tau}\phi_{12} \\ x_2 &= C_1 e^{-i\mu_1\tau}\phi_{21} + C_2 e^{-i\mu_2\tau}\phi_{22} \end{aligned} \tag{III-6}$$

Form II. $(\mu = \mu_1 = \mu_2 + n$, n any integer or zero)

When $\mu_1 = \mu_2 + n$, there are two possible forms of solution. For one, the Floquet modes are

$$\{x_1 = e^{-i\mu\tau}\phi_{11} , \quad x_2 = e^{-i\mu\tau}\phi_{21}\} \tag{III-7}$$

and

$$\{x_1 = e^{-i\mu\tau}\phi_{12} , \quad x_2 = e^{-i\mu\tau}\phi_{22}\} \tag{III-8}$$

These may be combined to form the general solution.

$$x_1 = e^{-i\mu\tau}(C_1\phi_{11} + C_2\phi_{12})$$
$$x_2 = e^{-i\mu\tau}(C_1\phi_{21} + C_2\phi_{22}) \qquad \text{(III-9)}$$

<u>Form III. ($\mu = \mu_1 = \mu_2 + n$, n any integer or zero)</u>

For the other type of solution corresponding to $\mu_1 = \mu_2 + n$, the Floquet modes are

$$\{x_1 = e^{-i\mu\tau}\phi_{11} \ , \quad x_2 = e^{-i\mu\tau}\phi_{21}\} \qquad \text{(III-10)}$$

and

$$\{x_1 = e^{-i\mu\tau}[\tau\phi_{11} + \phi_{12}] \ , \quad x_2 = e^{-i\mu\tau}[\tau\phi_{21} + \phi_{22}]\} \qquad \text{(III-11)}$$

which may be combined to form the general solution which can satisfy arbitrary initial conditions.

$$x_1 = e^{-i\mu\tau}(C_1\phi_{11} + C_2[\tau\phi_{11} + \phi_{12}])$$
$$x_2 = e^{-i\mu\tau}(C_1\phi_{21} + C_2[\tau\phi_{21} + \phi_{22}]) \qquad \text{(III-12)}$$

Notice that the "Form III" solutions contain terms linear in τ . No such terms appear in the "Form I" or "Form II" solutions.

We wish to state at this point some theorems which will be useful in later stages of the report and which will give us some information in addition to the bare-boned Floquet results.

Relationship between Any Two Solutions

The first result we wish to state gives a relationship between any two solutions. Assume we have found two solutions to (III-1). If we form the quantity $D(\tau)$ defined by

$$D(\tau) = x_{11}(\tau)x_{22}(\tau) - x_{12}(\tau)x_{21}(\tau) ,$$

then in accord with Theorem I in Appendix A, we have the useful result

$$D(\tau) = D(\tau_0)\exp\left[\int_{\tau_0}^{\tau} (\theta_{11}(\tau') + \theta_{22}(\tau'))d\tau'\right] \qquad \text{(III-13)}$$

If we apply (III-13) to (II-4) and (II-5) and let $\tau_0 = 0$, we find that

$$D(\tau) = D(0)\exp[-i\varepsilon\tau - \delta\tau - 2i\beta\sin\tau] \qquad \text{(III-14)}$$

The proof (III-13) is very simple and merely involves differentiating $D(\tau)$ to find

$$\frac{dD(\tau)}{d\tau} = D(\tau)(\theta_{11}(\tau) + \theta_{22}(\tau)) .$$

This is a differential equation for $D(\tau)$ which may be immediately solved to give (III-13).

From Eq. (III-14) it follows that for finite values of τ, $D(\tau)$ can only be zero if $D(0) = 0$. Furthermore, if $D(0) = 0$, then $D(\tau)$ is zero for all times. Thus, if two particular solutions, $\{x_{11}(\tau), x_{21}(\tau)\}$ and $\{x_{12}(\tau), x_{22}(\tau)\}$, correspond to a non-vanishing value for $D(0)$, they form a fundamental set of solutions to Eqs. (II-4) and (II-5).

The Normalization Equation

We wish to now consider the function $A(\tau)$ which is defined by:

$$A(\tau) = x_1^*(\tau)x_1(\tau) + x_2^*(\tau)x_2(\tau)$$

$\{x_1(\tau), x_2(\tau)\}$ is <u>any</u> solution to equations (III-1). Differentiating $A(\tau)$ we find, in general,

$$\frac{dA(\tau)}{d\tau} = x_1^*x_1(\theta_{11} + \theta_{11}^*) + x_1^*x_2(\theta_{21}^* + \theta_{12}) + x_2^*x_2(\theta_{22} + \theta_{22}^*) + x_1x_2^*(\theta_{12}^* + \theta_{21})$$

For the special case of equations (II-4) and (II-5) for which $x_1 = a$ and $x_2 = b$, we have

$$\frac{d}{d\tau}[a^*(\tau)a(\tau) + b^*(\tau)b(\tau)] = -2\delta b^*(\tau)b(\tau) \qquad \text{(III-15)}$$

(III-15) tells us that for the case of $\delta = 0$, $A(\tau)$ is a constant for all time. When $\delta \neq 0$, this is not true.

Since $\Psi(\underset{\sim}{r},t)$ is given by Eq. (I-3) in terms of η_a and η_b which are given by Eqs. (II-1) and (II-2), the relationship between the normalization integral and $A(\tau) = a^*a + b^*b$ is

$$\int \Psi^*(\underset{\sim}{r},t)\Psi(\underset{\sim}{r},t)d\underset{\sim}{r} = \eta_a^*\eta_a + \eta_b^*\eta_b$$

$$= A(\tau)\exp[-(\gamma_a/\omega)\tau]$$

Thus, in order for the normalization to remain invariant with respect to time, it is necessary that, in addition to $\delta = 0$ (or $\gamma_a = \gamma_b$), that $\gamma_a = 0$. This is consistent with the statement that both γ_a and γ_b remove particles from both state a and state b .

Knowledge of A Second Linearly Independent Solution From Knowledge of Any Particular Solution: $\delta = 0$ and $\delta \neq 0$

Let us first rewrite equations (II-4) and (II-5) in the following manner:

$$\begin{aligned} \dot{a} &= -ifb \\ \dot{b} &= -[ig + \delta]b - ifa \end{aligned} \qquad \text{(III-16)}$$

$f(\tau)$ and $g(\tau)$ are defined in the following manner:

$$f(\tau) \;=\; 2\alpha\cos\tau\;; \qquad g(\tau) \;=\; \varepsilon + 2\beta\cos\tau\;.$$

We wish to consider (III-16) first when $\delta = 0$ and then when $\delta \neq 0$. Note that the results we derive will apply to any system in which $f(\tau)$ and $g(\tau)$ are real functions and δ is a real parameter.

Case I: $\delta = 0$

Suppose that when $\delta = 0$, we have found a particular solution to (III-16) which we will call $\{a_1,b_1\}$. We can immediately write down another linearly independent solution which we will call $\{a_2,b_2\}$. The second solution is given by

$$\begin{aligned} a_2 &= -\,b_1^* e^{-\int_0^\tau [ig]d\tau'} \\ b_2 &= a_1^* e^{-\int_0^\tau [ig]d\tau'} \end{aligned} \qquad \text{(III-17)}$$

From equation (III-17) it follows that

$$D(0) \;=\; a_1^*a_1 + b_1^*b_1 \;=\; A(0)$$

For the solutions of (II-4) and (II-5) where $g(\tau) = \varepsilon + 2\beta\cos\tau$ and $\delta = 0$, equation (III-17) becomes

$$\begin{aligned} a_2 &= -\,b_1^* e^{-i\varepsilon\tau - 2i\beta\sin\tau} \\ b_2 &= a_1^* e^{-i\varepsilon\tau - 2i\beta\sin\tau} \end{aligned} \qquad \text{(III-18)}$$

This second solution (III-17) may be derived by comparing (III-15) and (III-13). For this case of $\delta = 0$, equation (III-13) becomes

$$a_1(\tau)b_2(\tau) - b_1(\tau)a_2(\tau) = D(0)e^{-\int_0^\tau [ig]d\tau'} \qquad \text{(III-19)}$$

According to the normalization equation (equation (III-16)), we have, when $\delta = 0$,

$$a_1(\tau)a_1^*(\tau) + b_1(\tau)b_1^*(\tau) = A(0) \ .$$

$A(0)$ is some non-zero constant since we assume that $\{a_1(\tau), b_1(\tau)\}$ is a non-trivial solution. Multiplying both sides of the normalization equation by

$$(D(0)/A(0))\exp[-\int_0^\tau [ig]d\tau'] \ ,$$

we find:

$$\frac{D(0)}{A(0)} [a_1(\tau)a_1^*(\tau) + b_1(\tau)b_1^*(\tau)]e^{-\int_0^\tau [ig]d\tau'} = D(0)e^{-\int_0^\tau [ig]d\tau'}$$

(III-20)

Comparison of (III-20) with (III-19) demonstrates the validity of (III-17).

Case II: $\delta \neq 0$

Here we are considering (III-16) for the case of $\delta \neq 0$. Suppose that we have found a particular solution to (III-16) which we will call $\{a_1, b_1\}$. Form the functions $\{\underline{a}_1, \underline{b}_1\}$ by replacing δ wherever it appears in $\{a_1, b_1\}$ by $(-\delta)$. $\{\underline{a}_1, \underline{b}_1\}$ must obey the following equations:

$$\dot{\underline{a}}_1 = -if\underline{b}_1$$

$$\dot{\underline{b}}_1 = -[ig - \delta]\underline{b}_1 - if\underline{a}_1$$

We assert that another linearly independent solution to (III-16) is given by:

$$\begin{aligned} a_2 &= -(\underline{b}_1)^* \exp[-\int_0^\tau [ig + \delta] d\tau'] \\ b_2 &= (\underline{a}_1)^* \exp[-\int_0^\tau [ig + \delta] d\tau'] \end{aligned} \qquad \text{(III-21)}$$

as long as $g(\tau)$ and $f(\tau)$ may be expanded in a power series in τ for sufficiently small values of τ. For the case of equations (II-4) and (II-5) where $f(\tau) = 2\alpha\cos\tau$ and $g(\tau) = \varepsilon + 2\beta\cos\tau$ (here, therefore, both $f(\tau)$ and $g(\tau)$ can be expanded in power series in τ), equation (III-21) becomes

$$\begin{aligned} a_2(\tau) &= -(\underline{b}_1)^* \exp[-i\varepsilon\tau - \delta\tau - 2i\beta\sin\tau] \\ b_2(\tau) &= (\underline{a}_1)^* \exp[-i\varepsilon\tau - \delta\tau - 2i\beta\sin\tau] \end{aligned} \qquad \text{(III-22)}$$

The proof of (III-21) involves two steps. The first is showing that the solution, $\{a_2,b_2\}$ of equation (III-21), does indeed satisfy (III-16). This is shown by simple differentiation of (III-21) and utilization of the equations for $\dot{\underline{a}}_1$ and $\dot{\underline{b}}_1$.

The second step is showing that $\{a_1,b_1\}$ and $\{a_2,b_2\}$ are linearly independent. The linear independence is shown by proving that

$$a_1b_2 - b_1a_2 = [a_1(\underline{a}_1)^* + b_1(\underline{b}_1)^*]\exp[-\int_0^\tau [ig + \delta]d\tau'] \neq 0$$

Since g is by hypothesis pure real, the exponential term in the previous equation can certainly never equal zero for finite values of τ . The linear independence is therefore shown by demonstrating that

$$B(\tau) = a_1(\underline{a}_1)^* + b_1(\underline{b}_1)^* \neq 0 . \qquad \text{(III-23)}$$

Utilizing the differential equations for a_1, b_1, $\underline{a}_1$ and $\underline{b}_1$, we may easily show that the derivative of $B(\tau)$ with respect to τ is zero. Therefore,

$$a_1(\underline{a}_1)^* + b_1(\underline{b}_1)^* = \text{constant}$$

We must show that this constant is non-zero. This is done by looking at the solution to (III-16) when all quantities are expressed in their power series in τ . We therefore assume

$$f(\tau) = f^{(0)} + f^{(1)}\tau + f^{(2)}\tau^2 + \ldots$$

$$g(\tau) = g^{(0)} + g^{(1)}\tau + g^{(2)}\tau^2 + \ldots \qquad \text{(III-24)}$$

If we look for the particular solution for which $a(0) = a^{(0)}$, $b(0) = b^{(0)}$ where $a^{(0)}$ and $b^{(0)}$ are arbitrary complex numbers and both may not simultaneously be zero, for sufficiently small values of τ, we may write

$$a(\tau) = a^{(0)} + a^{(1)}\tau + a^{(2)}\tau^2 + \ldots$$

$$b(\tau) = b^{(0)} + b^{(1)}\tau + b^{(2)}\tau^2 + \ldots \qquad \text{(III-25)}$$

Using the expansions (III-24) and (III-25) in (III-16), we find that the resulting equations for the expansion coefficients, $a^{(n)}$ and $b^{(n)}$, may be solved in terms of the arbitrary constants $a^{(0)}$ and $b^{(0)}$ and the given values of δ, the $f^{(n)}$'s and the $g^{(n)}$'s. For instance,

$$a^{(1)} = - if^{(0)}b^{(0)}$$

$$b^{(1)} = - ig^{(0)}b^{(0)} - if^{(0)}a^{(0)} + \delta b^{(0)}$$

If some particular solution is

$$a = a^{(0)} + a^{(1)}\tau + \ldots$$
$$b = b^{(0)} + b^{(1)}\tau + \ldots \qquad \text{(III-26)}$$

by definition we have,

$$\underline{a} = a^{(0)} + a^{(1)}\tau + \ldots$$
$$\underline{b} = b^{(0)} + [b^{(1)} - 2\delta b^{(0)}]\tau + \ldots \qquad \text{(III-27)}$$

Using (III-26) and (III-27) in (III-23) we find that

$$a(\underline{a})^* + b(\underline{b})^* = a^{(0)}(a^{(0)})^* + b^{(0)}(b^{(0)})^* \qquad \text{(III-28)}$$

The term on the right-hand side of (III-28) can never be zero unless <u>both</u> $a^{(0)}$ and $b^{(0)}$ are zero. This situation, by hypothesis, cannot occur. Therefore, we have demonstrated that equations (III-21) and (III-22) give linearly independent second solutions.

"Form III" Solutions Can Never Occur for Equations (III-16)

Provided that the functions $f(\tau)$ and $g(\tau)$ which appear in (III-16) are periodic so that

$$f(\tau) = f(\tau + P) \ ; \quad g(\tau) = g(\tau + P) \ ,$$

the first Corollary of Appendix A tells us that there is <u>always</u> one particular solution to (III-16) of the form

$$a_1(\tau) = e^{-i\mu\tau}\phi_{a1}(\tau) , \quad b_1(\tau) = e^{-i\mu\tau}\phi_{b1}(\tau) . \qquad \text{(III-29)}$$

Here, μ is a constant and $\phi_i(\tau) = \phi_i(\tau + P)$ $(i = a1, b1)$. Certainly the functions in (III-29) have no terms linear in τ . According to equation (III-21), we can write down another linearly independent solution as

$$\begin{aligned} a_2(\tau) &= -e^{i\underline{\mu}^*\tau}\underline{\phi}^*_{b1}(\tau)\exp[-\int_0^\tau [ig + \delta]d\tau'] \\ b_2(\tau) &= e^{i\underline{\mu}^*\tau}\underline{\phi}_{a1}(\tau)\exp[-\int_0^\tau [ig + \delta]d\tau'] \end{aligned} \qquad \text{(III-30)}$$

The "barred" quantities are related to the "unbarred" quantities by replacing (δ) wherever it appears in the "unbarred" quantities by $(-\delta)$. Certainly, because of the way they have been defined, a_2 and b_2 can have no terms in them which are linear in τ . Since $\{a_1, b_1\}$ and $\{a_2, b_2\}$ are linearly independent, <u>all</u> solutions to (III-16) may be written as

$$a = C_1 a_1 + C_2 a_2$$

$$b = C_1 b_1 + C_2 b_2$$

C_1 and C_2 are arbitrary constants. Therefore, there are <u>no</u> solutions to (III-16) having terms linear in τ . We may therefore conclude that "Form III" solutions may never occur in equations (III-16).

The application of this present discussion to equations (II-4) and (II-5) is that these equations may never have "Form III" solutions. We cannot *à priori* tell, however, whether the solution is of "Form I" or "Form II." As later sections of this report will show, we have found "Form I" solutions to be the general rule, although we must allow for "Form II" solutions for certain "accidental" values of the parameters α, β, ε and δ .

The Characteristic Exponent for "Form II" Solutions

Let us assume that the Floquet Normal Mode solutions to (II-4) and (II-5) are of "Form II". We therefore have two linearly independent particular solutions:

$$a_1 = e^{-i\mu\tau}\phi_{a1}\ , \quad b_1 = e^{-i\mu\tau}\phi_{b1}$$

$$a_2 = e^{-i\mu\tau}\phi_{a2}\ , \quad b_2 = e^{-i\mu\tau}\phi_{b2}$$

μ is a constant and $\phi_{ij}(\tau) = \phi_{ij}(\tau + 2\pi)(i = a,b\ ,\ j = 1,2)$.

Substituting these solutions into (III-14), we have

$$[\phi_{a1}\phi_{b2} - \phi_{a2}\phi_{b1}]e^{-2i\mu\tau} = D(0)e^{[-i\varepsilon\tau-\delta\tau-2i\beta\sin\tau]} \qquad \text{(III-31)}$$

Since the term in brackets on the left-hand side of (III-31) has periodicity 2π as does $\exp[-2i\beta\sin\tau]$, we may equate the linear terms in the exponents in (III-31) to write the "Form II" characteristic exponent as

$$\mu = \frac{\varepsilon}{2} - i\,\frac{\delta}{2}$$

The Characteristic Exponents for "Form I" Solutions

If the solutions to (II-4) and (II-5) are "Form I" solutions, we may write two linearly independent solutions as

$$a_1 = e^{-i\mu_1\tau}\phi_{a1} , \quad b_1 = e^{-i\mu_1\tau}\phi_{b1}$$
$$a_2 = e^{-i\mu_2\tau}\phi_{a2} , \quad b_2 = e^{-i\mu_2\tau}\phi_{b2}$$

The μ's are constants and $\mu_1 \neq \mu_2 + n$ (n any integer or zero). The ϕ's are periodic with periodicity 2π .

Substituting these solutions into (III-14), we have:

$$[\phi_{a1}\phi_{b2} - \phi_{a2}\phi_{b1}]e^{-i(\mu_1+\mu_2)\tau} = D(0)e^{[-i\varepsilon\tau-\delta\tau-2i\beta\sin\tau]}$$

By the arguments we used above, we may write:

$$[\phi_{a1}\phi_{b2} - \phi_{a2}\phi_{b1}] = D(0)\exp[-2i\beta\sin\tau]$$

and

$$\mu_1 + \mu_2 = \varepsilon - i\delta \qquad \text{(III-32)}$$

<u>If $\delta = 0$, μ is Pure Real</u>

Write μ_1 and μ_2 in terms of their real and imaginary components:

$$\mu_1 = (\mu_1)_r + i(\mu_1)_i$$

$$\mu_2 = (\mu_2)_r + i(\mu_2)_i$$

From Eq. (III-32), when $\delta = 0$,

$$(\mu_1)_i = -(\mu_2)_i$$

Let the two Floquet Normal Modes be written according to:

$$a_j = e^{-i\mu_j\tau}\,\phi_{aj}$$

$$b_j = e^{-i\mu_j\tau}\,\phi_{bj}$$

where $j = 1$ or 2 . From Eqs. (III-18) we have:

$$e^{-i\mu_2\tau}\,\phi_{a2} = -e^{i(\mu_1)^*\tau}\,\phi_{b1}^*\,e^{-i\varepsilon\tau}\,e^{-2i\beta\sin\tau}$$

$$e^{-i\mu_2\tau}\,\phi_{b2} = e^{i(\mu_1)^*\tau}\,\phi_{a1}^*\,e^{-i\varepsilon\tau}\,e^{-2i\beta\sin\tau}$$

Comparing left- and right-hand sides of the above equations, we have:

$$\mu_2 = -(\mu_1)^* + \varepsilon$$

Since ε is by definition pure real,

$$(\mu_2)_i = (\mu_1)_i$$

If it is true that both

$$(\mu_1)_i = -(\mu_2)_i \quad \text{and} \quad (\mu_1)_i = (\mu_2)_i$$

then it must be true that

$$(\mu_1)_i = (\mu_2)_i = 0$$

and therefore, <u>if the Floquet Normal Mode solutions are defined according to</u>

$$a_j = e^{-i\mu_j\tau}\,\phi_{aj}$$

$$b_j = e^{-i\mu_j\tau}\,\phi_{bj} \qquad j = 1,2$$

<u>when $\delta = 0$, μ_j is pure real. When $\delta \neq 0$, μ_j will, in general, be complex.</u>

Exact Solutions in Terms of Fourier Coefficients

The Poincaré-Floquet theory has been used to derive complicated but exact solutions to (II-4) and (II-5) by taking advantage of the fact that the Floquet Form of solution is a periodic function multiplying an exponential function. Since we may write the solution to (II-4) and (II-5) as

$$a(\tau) = \phi_a(\tau)e^{-i\mu\tau}$$
$$b(\tau) = \phi_b(\tau)e^{-i\mu\tau} \qquad \text{(III-33)}$$

where μ is a constant and $\phi_j(\tau + 2\pi) = \phi_j(\tau)$, we may further, by using Fourier's Theorem, write,

$$\phi_a(\tau) = \sum_{j=-\infty}^{\infty} A_j e^{ij\tau} \;; \quad \phi_b(\tau) = \sum_{j=-\infty}^{\infty} B_j e^{ij\tau} \qquad \text{(III-34)}$$

Substituting (III-33) and (III-34) into (II-4) and (II-5), we obtain an algebraic equation of the form

$$(\underset{\approx}{M} - \mu\underset{\approx}{I})\underset{\sim}{C} = 0 \,. \qquad \text{(III-35)}$$

Here μ is the characteristic exponent of expressions (III-33), $\underset{\sim}{I}$ is the infinite unit matrix, $\underset{\approx}{M}$ is an infinite square matrix the elements of which involve the parameters ε, δ, α and β as well as integers. $\underset{\sim}{C}$ is an infinite column matrix whose elements are the Fourier expansion coefficients. M has double indices so that a typical element is $M_{k,\ell;k',\ell'}$ where k or k' is either A or B and ℓ or ℓ' is any (positive or negative) integer or zero. Thus A,n represents A_n and the double indices are used to avoid the printing difficulty of a subscript on a subscript. The matrix elements of $\underset{\approx}{M}$ are

$$
\begin{aligned}
(\underset{\approx}{M})_{A,j;A,j} &= j \\
(\underset{\approx}{M})_{B,j;B,j} &= j + \varepsilon - i\delta \\
(\underset{\approx}{M})_{A,j;B,j\pm 1} &= \alpha = (\underset{\approx}{M})_{B,j;A,j\pm 1} \\
(\underset{\approx}{M})_{B,j;B,j\pm 1} &= \beta
\end{aligned}
\qquad \text{(III-36)}
$$

It is convenient to write the rows or columns in the order

$$... \ A,n; \ B,n; \ A,n-1; \ B,n-1; \ ...$$

(III-35) is explicitly written out in equation (V-5) of this report.

In order that there be a solution to (III-35) it is necessary that

$$\det|\underset{\approx}{M} - \mu\underset{\approx}{I}| = 0 \qquad \text{(III-37)}$$

Note that (III-37) is an infinite secular equation which must be solved to find μ . Once μ is known, the Fourier coefficients A_j and B_j may be computed and thus the problem is solved.

From equation (III-37) of this section, we know that if the solution is of Form I, once we know μ_1 , we can immediately write down μ_2 . The elements of $\underset{\approx}{M}$ are given by (III-36) and if we look at (V-5) we see the infinite, square $\underset{\approx}{M}$ matrix explicitly written out. Inspection of $\underset{\approx}{M}$ and consideration of equation (III-37) leads us to this important result which is also stated in Appendix A: <u>if μ_1 is a solution to (III-37), so is $\mu_1 + n$ where n is any integer including zero</u>. The proof of this statement is simple. Because of the periodic nature of the infinite matrix $\underset{\approx}{M}$, $(\underset{\approx}{M} - \mu_1\underset{\approx}{I})$ is the same infinite matrix as $(\underset{\approx}{M} - (\mu_1 + n)\underset{\approx}{I})$.

Four numerical methods for finding the characteristic exponents have been proposed. These are useful when the values of ε, δ, α and β are such that we are unable to find perturbation solutions.

Meadows (1962) and Ashby (1968) have shown, that for the two-level problem, equation (III-37) may be manipulated to obtain a simple transcendental equation for μ which involves an infinite determinant which depends only on ε, δ, α, β and known integers. This infinite determinant is closely related, but not identical to the determinant of the matrix $\underset{\approx}{M}$ of equation (III-37). So if this determinant is evaluated, μ may be exactly computed.

We give more details concerning this method in Chapter XVI where we describe how the Meadows-Ashby method can be used to find numerical values for the characteristic exponents. The application of this method to more complicated problems is found in Ashby's (1968) article and in Ross's (1969) thesis.

Autler and Townes (1955) have obtained an exact formal solution of equations (II-4) and (II-5) for the case of $\delta = \beta = 0$. Starting with (III-35), they obtain an equation for μ in terms of two infinite continued fractions which themselves depend on μ. In Chapter XVII we trivially extend their work to include non-vanishing δ and describe how their formulas are used to numerically find μ. Unfortunately, their technique cannot be extended to take into account non-vanishing β.

When $\delta = \beta = 0$, equation (III-35) reduces to the problem of finding the eigenvalues and eigenvectors of a real, symmetric tri-diagonal matrix. A direct numerical attack of this latter problem is discussed in Chapter XVIII.

Shirley (1963) utilized equation (A-12) (see Appendix A) to obtain numerical values of the characteristic exponents. The basic input into (A-12) is the result of a numerical solution to equations (II-4) and (II-5). We discuss this technique and the simplifications which arise when either δ or β (or both) vanish in Chapter XIX.

None of the four techniques mentioned above are useful in obtaining formal perturbation solutions since such results obtained from them can be more easily obtained by more familiar and more direct methods. The four techniques are however important, since in the regimes where we have not been able to find simple perturbation solutions, recourse must be made to one of the four techniques mentioned above to find numerical solutions of the problem.

IV. LIMITS IN WHICH EXACT SOLUTIONS ARE KNOWN

Although we do not know the exact solution of (II-4) and (II-5) in terms of elementary functions, we can solve (II-4) and (II-5) in the following three limits:

(A) $\alpha \to 0$

(B) $\varepsilon \to 0$ and $\delta \to 0$

(C) $\omega \to 0$

Case (A): $\alpha \to 0$

Here equations (II-4) and (II-5) become uncoupled and are solved by simple quadrature to obtain

$$a(\tau) = a(0)$$

$$b(\tau) = b(0)\exp[-i\varepsilon\tau - \delta\tau - 2i\beta\sin\tau]$$

Case (B): $\varepsilon \to 0$ and $\delta \to 0$

For this case, we can solve the resulting equations by changing the independent variable to $z = \sin\tau$. Doing this we obtain

$$da/dz = -2i\alpha b$$

$$db/dz = -2i\beta b - 2i\alpha a \qquad \text{(IV-1)}$$

Equations (IV-1) are simultaneous, homogeneous first order differential equations with constant coefficients which may be easily solved* to give

$$a(\tau) = C_1 e^{-i\lambda_+ \sin\tau} + C_2 e^{-i\lambda_- \sin\tau}$$
$$b(\tau) = (2\alpha)^{-1}[C_1\lambda_+ e^{-i\lambda_+ \sin\tau} + C_2\lambda_- e^{-i\lambda_- \sin\tau}] \qquad \text{(IV-2)}$$

C_1 and C_2 are arbitrary constants and $\lambda_\pm$ is defined by

$$\lambda_\pm = \beta \pm (\beta^2 + 4\alpha^2)^{1/2} \qquad \text{(IV-3)}$$

Case (C): $\omega \to 0$

In this case, $\cos\omega t$ in equation (I-1) should be replaced by unity. Thus, transforming the independent variable back from τ to t, (II-4) and (II-5) become:

$$da/dt = -2iFV_{ab}b$$
$$db/dt = -2iFV_{ab}a - i[(W_b - W_a) - \tfrac{1}{2}i(\gamma_b - \gamma_a) + 2F(V_{bb} - V_{aa})]b \qquad \text{(IV-4)}$$

(IV-4) and (IV-1) are the same type of differential equation system and we may easily solve (IV-4) to obtain:

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* See Protter (1964) and Morrey, Chap. 16, Sect. 10, or any book on ordinary differential equations.

$$a = C_1 e^{-i\lambda_+' t} + C_2 e^{-i\lambda_-' t}$$
$$b = (2FV_{ab})^{-1}[\lambda_+' C_1 e^{-i\lambda_+' t} + C_2 \lambda_-' e^{-i\lambda_-' t}] \qquad \text{(IV-5)}$$

where

$$\lambda_\pm' = \tfrac{1}{2}[q \pm (q^2 + 16F^2(V_{ab})^2)^{1/2}]$$

and

$$q = (W_b - W_a) - \tfrac{i}{2}(\gamma_b - \gamma_a) + 2F(V_{bb} - V_{aa}) \qquad \text{(IV-6)}$$

We have briefly mentioned these solvable limits since the solutions obtained in these limits will form the zeroth order starting points of the perturbation techniques which we will use in the remainder of this report.

V. TRANSFORMATION OF THE TIME-DEPENDENT PROBLEM TO A TIME-INDEPENDENT QUANTUM MECHANICAL PROBLEM

In section III of this report, we transformed the time-dependent problem of equations (II-4) and (II-5) into a time-independent eigenvalue-eigenvector problem which is succinctly stated by (III-35). In this section we wish to restate the latter algebraic problem of determining the value of the eigenvalue μ and its corresponding A_n, B_n eigenvectors in terms of well-known quantum mechanical stationary state perturbation techniques using Dirac's bra-ket notation to represent the Fourier coefficients. The matrix $\underset{\sim}{M}$ of (III-35) will correspond to the matrix of a Hamiltonian H_F, μ will correspond to the energy of the system and (V-5) will become the system's secular equation. As we will see, H_F is a non-hermitian operator. This fact has caused us no difficulty in subsequent sections of this report. Doing this, we will be in effect showing that the original time-dependent problem is equivalent to a stationary-state quantum mechanical problem and we may then apply all of the powerful, well-known perturbation techniques which are utilized to solve this latter type of problem.

We should first recall that in section III we used Floquet's Theorem (equation (III-33)) and Fourier's Theorem (equation (III-34)) to obtain the algebraic equation given in (III-35). Following Shirley (1963,1965), we can manufacture the following stationary-state quantum mechanical problem which is equivalent to the problem expressed in (III-35).

First define a basis $|k,n\rangle$ such that the index k can be either A or B. Let the index n range from $-\infty$ to ∞ and let the basis be orthonormal, i.e.,

$$\langle k,n|\ell,m\rangle = \delta_{k,\ell}\delta_{n,m} \tag{V-1}$$

The "deltas" on the right-hand side (V-1) are "Krönecker deltas" and are not to be confused with the parameter δ which has no subscripts on it.

Define the non-hermitian Floquet Hamiltonian, H_F, so that

$$\begin{aligned} H_F|A,j\rangle &= j|A,j\rangle + \alpha[|B,j+1\rangle + |B,j-1\rangle] \\ H_F|B,j\rangle &= (j+\varepsilon-i\delta)|B,j\rangle + \alpha[|A,j+1\rangle + |A,j-1\rangle] \\ &\quad + \beta[|B,j+1\rangle + |B,j-1\rangle] \end{aligned} \tag{V-2}$$

If we ask "what are the eigenvalues of H_F", we are, in effect, asking for the solutions to the Schrödinger-type equation

$$H_F|\mu\rangle = \mu|\mu\rangle \tag{V-3}$$

where μ is an eigenvalue of H_F and $|\mu\rangle$ is the associated eigenvector. The function $|\mu\rangle$ can be expressed as a linear combination of the complete set of basis functions $|A,j\rangle$ and $|B,j\rangle$ so that

$$|\mu\rangle \;=\; \sum_{j=-\infty}^{\infty} (A_j|A,j\rangle + B_j|B,j\rangle) \qquad \text{(V-4)}$$

where the A_j's and B_j's are expansion coefficients. Substituting (V-4) into (V-3), we may multiply the resulting equation in turn by each and every bra $\langle k',n'|$. Doing this we are led to equation (V-5) which is the matrix representation of the following set of equations:

$$\sum_{k,n} \langle k',n'|H_F|k,n\rangle\langle k,n|\mu\rangle - \mu\langle k',n'|\mu\rangle \;=\; 0$$
$$k' = A \text{ or } B\;; \quad n' = -\infty \text{ to } \infty\,. \qquad \text{(V-6)}$$

Here the $\langle k',n'|H_F|k,n\rangle$ correspond to the elements of $\underset{\approx}{M}$ and the $\langle k,n|\mu\rangle$ correspond to the elements of the column vector $\underset{\sim}{C}$ in equation (III-35).

After we have found an eigenvalue, μ , of H_F and after we have found the expansion coefficients A_j and B_j , the time-dependent functions $a(\tau)$ and $b(\tau)$ may be recovered by the following relationships:

$$a(\tau) \;=\; e^{-i\mu\tau} \sum_{j=-\infty}^{\infty} A_j e^{ij\tau} \qquad \text{(V-7)}$$

$$b(\tau) \;=\; e^{-i\mu\tau} \sum_{j=-}^{\infty} B_j e^{ij\tau} \qquad \text{(V-8)}$$

$$
\begin{vmatrix}
 & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\
\cdots & 2 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\
\cdots & 0 & 2+\varepsilon-i\delta & \alpha & \beta & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\
\cdots & 0 & \alpha & 1 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & \cdots \\
\cdots & \alpha & \beta & 0 & 1+\varepsilon-i\delta & \alpha & \beta & 0 & 0 & 0 & 0 & \cdots \\
\cdots & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & \alpha & 0 & 0 & \cdots \\
\cdots & 0 & 0 & \alpha & \beta & 0 & \varepsilon-i\delta & \alpha & \beta & 0 & 0 & \cdots \\
\cdots & 0 & 0 & 0 & 0 & 0 & \alpha & -1 & 0 & 0 & \alpha & \cdots \\
\cdots & 0 & 0 & 0 & 0 & \alpha & \beta & 0 & -1+\varepsilon-i\delta & \alpha & \beta & \cdots \\
\cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha & -2 & 0 & \cdots \\
\cdots & 0 & 0 & 0 & 0 & 0 & 0 & \alpha & \beta & 0 & -2+\varepsilon-i\delta & \cdots \\
 & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots &
\end{vmatrix}
\begin{vmatrix} \vdots \\ A_2 \\ B_2 \\ A_1 \\ B_1 \\ A_0 \\ B_0 \\ A_{-1} \\ B_{-1} \\ A_{-2} \\ B_{-2} \\ \vdots \end{vmatrix}
= \mu
\begin{vmatrix} \vdots \\ A_2 \\ B_2 \\ A_1 \\ B_1 \\ A_0 \\ B_0 \\ A_{-1} \\ B_{-1} \\ A_{-2} \\ B_{-2} \\ \vdots \end{vmatrix}
\qquad (V-5)
$$

VI. SUMMARY OF AND GUIDE TO THE REMAINING SECTIONS

In the remainder of this report we are concerned with finding and justifying perturbation solutions to Eqs. (II-4) and (II-5). Since no one perturbation scheme is useful for arbitrary values of α, β, δ and ε, we find that each range of values for α, β, δ and ε has associated with it, its own appropriate perturbation scheme. We shall explain nine different perturbation schemes which lead to converging, approximate expressions for the Floquet Normal Mode particular solutions. We will call these schemes Technique T1, Technique T2, etc. For certain ranges of the parameters no perturbation solutions to (II-4) and (II-5) have been found. In these instances we will have to resort to one of four numerical methods of solution which we will call T10,...,T14.

In Figures (VI-A) and (VI-B), we have drawn a flow chart which tells what technique to use for any values of the reduced parameters α, β, δ and ε. To use it, one must first specify the values of ε, δ, α and β. In these charts, ε_{min} is defined as the integer which is closest to ε:

$$0 \leq |\varepsilon_{min} - \varepsilon| \leq \tfrac{1}{2} .$$

(If ε is half-integer, ε_{min} could have either of two values.) If α and β are both much smaller than unity we must specify N where N

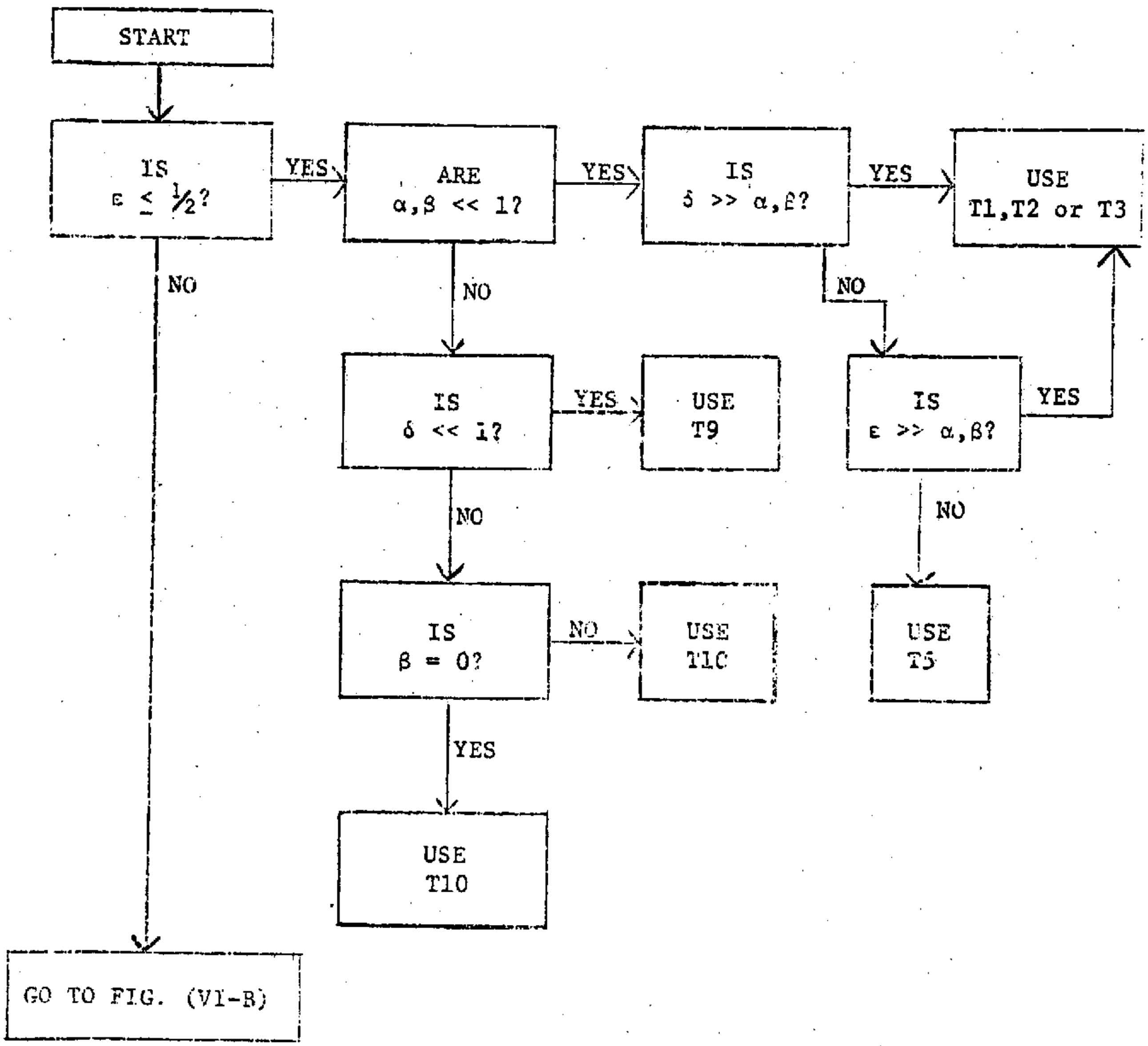

FIGURE (VI-A). Best techniques to use to obtain $a(\tau)$ and $b(\tau)$ for any values of the parameters α, β, δ and ε .

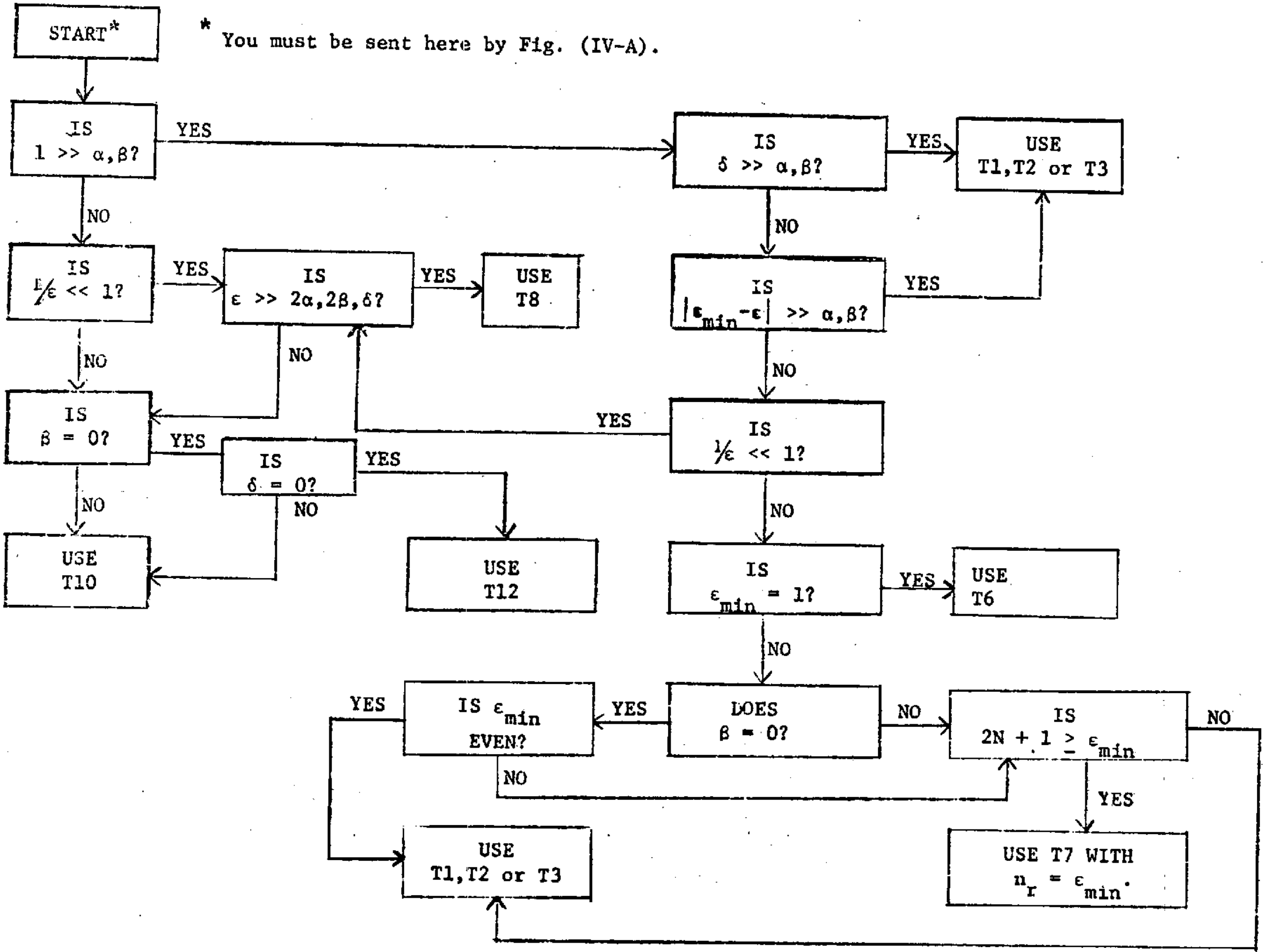

FIGURE (VI-B). Continuation of Fig. (VI-A). ε_{min} is the integer closest to ε, $0 \leq |\varepsilon_{min} - \varepsilon| \leq \frac{1}{2}$. N is the order of field strength (F^N) through which we require $a(\tau)$ and $b(\tau)$ to be accurate.

is the order of field strength (F^N) through which we want the "ϕ-parts" of the Floquet Normal Modes to be accurate.

The flow chart has been drawn so that when more than one technique is applicable, the reader is led to the preferred technique. When no one technique is clearly superior, the end box in the flow chart indicates all the techniques which may be used.

In Table VI we indicate the names of the techniques, their locations in the appropriate chapter of this report and the ranges for which the techniques give quickly converging perturbation solutions. By inspecting Table VI we can see that the techniques overlap. For example, if α, β , δ and ε are all much less than unity we could use either T9 or T5 to obtain approximate solutions.

TABLE VI. The descriptive names of the techniques, their locations in this report and their ranges of applicability.

Technique	Name	Location	Range of Applicability
T1	Non-degenerate Rayleigh-Schrödinger Field Strength Expansion	VIII	Either $\alpha,\beta \ll 1$; $\delta \gg \alpha,\beta$ ε arbitrary or $\alpha,\beta \ll 1$; $\lvert\varepsilon_{min} - \varepsilon\rvert \gg \alpha,\beta$ δ arbitrary
T2	Sen Gupta's Technique	VIII	(same as T1)
T3	Field Strength Expansion of Quotient Equations	VIII	(same as T1)
T4	Steady State Perturbation Theory	VIII	$\delta = \gamma_a = \gamma_b = 0$, $\alpha,\beta \ll 1$ $\lvert\varepsilon_{min} - \varepsilon\rvert \gg \alpha,\beta$
T5	Degenerate Rayleigh-Schrödinger Field Strength Expansion	IX	$\alpha,\beta,\varepsilon,\delta \ll 1$
T6	Partitioning Theory for the Main Resonance	XI	$\varepsilon \approx 1$; $\alpha,\beta,\delta \ll 1$
T7	Partitioning Theory for the Subharmonic Resonances	XII	$\varepsilon \approx n_r$; n_r = any integer greater than 1; $\alpha,\beta,\delta \ll 1$
T8	$(1/\varepsilon)$ Expansion of Quotient Equations	XIII	$\varepsilon \gg 1$; $\varepsilon \gg 2\alpha,2\beta,\delta$
T9	The $(\varepsilon - i\delta)$-expansion	XIV	$\varepsilon,\delta \ll 1$; α and β arbitrary
T10	Meadows-Ashby Technique	XVI	$\alpha,\beta,\delta,\varepsilon$ arbitrary
T11	Autler-Townes Technique	XVII	$\beta = 0$; $\alpha,\delta,\varepsilon$ arbitrary

Technique	Name	Location	Range of Applicability
T12	Numerical Diagonalization of a Real, Symmetric Tridiagonal Matrix	XVIII	$\beta = \delta = 0$; ε, α arbitrary
T13	Numerical Solution of Eqs. (II-4) and (II-5)	XIX	$\alpha, \beta, \delta, \varepsilon$ arbitrary

VII. POWER SERIES EXPANSIONS IN THE FIELD STRENGTH, F

In this section we consider expanding the solutions to equations (II-4) and (II-5) in powers of the field strength F . This can be accomplished by solving (V-3) by non-degenerate Rayleigh-Schrödinger Perturbation Theory.* This would first involve splitting up H_F in the following manner:

$$H_F = H_F^{(0)} + \lambda H_F^{(1)} \qquad \text{(VII-1)}$$

where λ is an ordering parameter which is set equal to unity. We will split up H_F so that the zeroth order Hamiltonian, $H_F^{(0)}$, is defined by

$$\begin{aligned} H_F^{(0)}|A,j\rangle &= j|A,j\rangle \\ H_F^{(0)}|B,j\rangle &= (j + \varepsilon - i\delta)|B,j\rangle \end{aligned} \qquad \text{(VII-2)}$$

The kets $|k,n\rangle$ (defined in Section V) are non-degenerate eigenfunctions of $H_F^{(0)}$. This non-degeneracy is strict as long as δ is non-vanishing.

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* A good concise treatment of non-degenerate Rayleigh-Schrödinger Perturbation Theory is given in Chap. VII of Schiff's (1955) book. For a more detailed treatment see the Hirschfelder (1964), Byers-Brown, Epstein review article.

<u>If</u> δ vanishes <u>and if</u> ε equals some integer, k (this corresponds to a resonance frequency), then accidental degeneracies may occur (i.e. in such a situation $|A,j\rangle$ and $|B,j-k\rangle$ would be degenerate). When ε is nearly (or exactly) equal to an integer and $\delta \approx 0$ so that the zeroth order is almost (or exactly) doubly degenerate, partitioning perturbation techniques (which are more generally applicable than Rayleigh-Schrödinger techniques) can be used to obtain a solution (Certain, Hirschfelder (1970a)). This is discussed in Section IX.

The $H_F^{(0)}$ is Hermitian when $\delta = 0$, but it is non-Hermitian when $\delta \neq 0$. In the case that $\delta \neq 0$,

$$\langle k',n'|H_F^{(0)}|k,n\rangle = \langle k,n|H_F^{(0)}|k',n'\rangle$$

but

$$\langle k',n'|(H_F^{(0)})^*|k,n\rangle \neq \langle k,n|H_F^{(0)}|k',n'\rangle ,$$

The $H_F^{(1)}$ is defined by

$$\begin{aligned} H_F^{(1)}|A,j\rangle &= \alpha[|B,j+1\rangle + |B,j-1\rangle] \\ H_F^{(1)}|B,j\rangle &= \alpha[|A,j+1\rangle + |A,j-1\rangle] + \beta[|B,j+1\rangle + |B,j-1\rangle] \end{aligned} \qquad \text{(VII-3)}$$

Note that the operator $H_F^{(1)}$ depends only upon the parameters α and β, therefore in terms of the "non-reduced" parameters, the split-up of the hamiltonian which is described by (VII-2) and (VII-3) is equivalent to a perturbation expansion in the field strength, F . $H_F^{(1)}$, unlike $H_F^{(0)}$, is a hermitian operator.

The usual non-degenerate Rayleigh-Schrödinger perturbation theory assumes that we may find the solutions to

$$H_F|\mu\rangle = \mu|\mu\rangle \qquad \text{(VII-4)}$$

by expanding both μ and $|\mu\rangle$ as power series in the ordering parameter λ , i.e.,

$$|\mu\rangle = \sum_{n=0}^{\infty} \lambda^n |\mu^{(n)}\rangle \qquad \text{(VII-5)}$$

$$\mu = \sum_{n-0}^{\infty} \lambda^n \mu^{(n)} \qquad \text{(VII-6)}$$

$|\mu^{(0)}\rangle$ would, of course, be one of the $|k,n\rangle$ kets. Substituting (VII-5), (VII-6) and (VII-1) into (VII-4), we may group together all terms proportional to λ^n , set them equal to zero and solve the resulting equations. For instance, a zeroth order equation is

$$H_F^{(0)}|k,n\rangle = \mu_{k,n}^{(0)}|k,n\rangle$$

where $\mu_{k,n}^{(0)}$ is the zeroth order non-degenerate eigenvalue of $|k,n\rangle$.

Let us suppose that we are seeking the perturbed wavefunction which arises from the zeroth order ket $|k_0,n_0\rangle$. Therefore

$$H_F^{(0)}|k_0,n_0\rangle = \mu_{k_0,n_0}^{(0)}|k_0,n_0\rangle$$

where

$$|k_0,n_0\rangle = |\mu_0^{(0)}\rangle .$$

The higher order corrections to $|k_0,n_0\rangle$, call them $|\mu_0^{(m)}\rangle$ $(m \geq 1)$, may be expressed in terms of the spectrum of the unperturbed hamiltonian, $H_F^{(0)}$;

$$|\mu_0^{(m)}\rangle = \sum_{k=A,B}{}' \sum_{j=-\infty}^{\infty}{}' C_{k,j}^{(m)}|k,j\rangle \qquad \text{(VII-7)}$$

where the $C_{k,j}^{(m)}$'s are the expansion coefficients and the primes on the summations indicate that the state $|k_0,n_0\rangle$ is to be excluded. This exclusion is perfectly all right if we stipulate that

$$\langle k_0,n_0|\mu_0^{(m)}\rangle = 0 \qquad m \geq 1$$

This stipulation, in the jargon of perturbation theory, is usually called "intermediate normalization." The point we wish to stress is that the expansion coefficients* in (VII-7) are always products of terms of the form:

$$G = \frac{\langle k,n|H_F^{(1)}|k',n'\rangle}{\mu_{k,n}^{(0)} - \mu_{k_0,n_0}^{(0)}} \qquad \text{(VII-8)}$$

where $k_0,k,k' = A$ or B , n_0,n,n' = any integer or zero with the stipulation that if k equals k_0 then n may not equal n_0 .

We wish to use (VII-8) in postulating a crude criterion of when a non-degenerate Rayleigh-Schrödinger series should quickly converge. The rule of thumb is this: the series should quickly converge if $H_F^{(0)}$ and $H_F^{(1)}$ are chosen so that G (defined by (VII-8)) will always be much less than unity. We say this, since, if G is always much less than unity then we can be sure that the component of the zeroth order ket, $|k,n\rangle$, in the m-th order correction, $|\mu_0^{(m)}\rangle$, will be smaller and smaller as m gets larger and larger. We will further assume that if the wavefunction is quickly converging, the energy will also quickly converge. Our criterion is hardly sophisticated, but we will take it as a working postulate.

If we now ask, "Under what conditions will a non-degenerate Rayleigh-Schrödinger perturbation treatment converge if H_F is split up according to (VII-2) and (VII-3)?" , we can answer this by looking at

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* See equations (II.17), (II.18) and (II.19) in Hirschfelder's (1964) review.

(VII-8) and by trying to determine the conditions under which G will be small. It will certainly be small if the magnitude of the denominator is much larger than the magnitude of the numerator.

Case I: $k = k_0 = A$ or B, $n \neq n_0$

If $k = k_0 = A$ or B, then from equation (VII-2), we can see that since n can never equal n_0, the quantity

$$\mu_{k,n}^{(0)} - \mu_{k_0,n_0}^{(0)}$$

will be some (positive or negative) integer. It's smallest magnitude is therefore unity. Since the numerator of G can only be α, β or 0 when its denominator must be unity or larger, we get the first requirement for the quick convergence of the non-degenerate Rayleigh-Schrödinger perturbation series, namely:

$$\underline{\text{both } \alpha \text{ and } \beta \ll 1} \qquad \text{(VII-9)}$$

Case II: $k \neq k_0$; $n = n_0$

If $k \neq k_0$ and $n = n_0$, the magnitude of the denominator of G will be $|\varepsilon - i\delta|$. The numerator of G will be α, β or 0. Thus, in addition to the requirement that α and β be much less than unity, we must impose the condition

$$\underline{\text{both } \alpha \text{ and } \beta \ll |\varepsilon - i\delta|} \qquad \text{(VII-10)}$$

for the non-degenerate Rayleigh-Schrödinger series to quickly converge.

Case III: $k \neq k_0$; $n \neq n_0$

This is the last possibility we must consider. Again, the numerator of G can either be α, β or 0 . The denominator of G for this case is

$$(n - n_0 \pm (\varepsilon - i\delta))$$

where the plus sign is taken if $k = B$ and the minus sign is taken otherwise. The quantity $(n - n_0)$ may never equal zero. We therefore obtain the last requirement for the quick convergence of the perturbation series:

$$\underline{\text{both } \alpha \text{ and } \beta << |n - n_0 \pm (\varepsilon - i\delta)|} \qquad \text{(VII-11)}$$

where $(n - n_0)$ is some non-zero integer. We may combine (VII-11) and (VII-10) into one expression and therefore conclude that the non-degenerate Rayleigh-Schrödinger perturbation series will quickly converge if both of the following conditions are satisfied

both α and $\beta << 1$ (VII-12a)

and α and $\beta << |N - \varepsilon + i\delta|$ where N is any integer or zero. (VII-12b)

To determine the ranges of parameters for which (VII-12b) holds, we should first recall that the complex quotient

$$\frac{y}{Z_r + iZ_i} = q_r + iq_i$$

where y, Z_r, Z_i, q_r and q_i are all real numbers will be small (i.e. both q_r and q_i will be much less than unity) if

(a) $Z_r >> y$

(b) $Z_i >> y$

(c) both Z_r and Z_i are much great than y .

Next define K_{min} to be the integer which makes the quantity $|K_{min} - \varepsilon|$ as small as possible. K_{min} could be zero, if $\varepsilon < 0.5$. If ε is half integer then there is a trivial ambiguity in K_{min} . In any case, K_{min} has been defined so that for a given value of ε , $0 \leq |K_{min} - \varepsilon| \leq 0.5$.

With this definition of K_{min} , we can say that the non-degenerate Rayleigh-Schrödinger perturbation series will quickly converge if either condition (a) or condition (b) is fulfilled:

(a) both α and $\beta << 1$; $\delta >> \alpha$ and β ; ε arbitrary.

(b) both α and $\beta << 1$; $|K_{min} - \varepsilon| >> \alpha$ and β ; δ arbitrary. K_{min} is the integer which makes $|K_{min} - \varepsilon|$ as small as possible.

(VII-13)

If the conditions given by (VII-13) are not met, then other techniques must be used. These other techniques form the basis for the rest of this report.

VIII. FOUR FIELD STRENGTH EXPANSIONS

In this section we discuss four techniques for expanding the Floquet Normal Modes in a series expansion in powers of the field strength F.

In "Technique T1" the non-degenerate Rayleigh-Schrödinger perturbation theory is used in terms of the bras and kets which we introduced in Section V and which are related to the Fourier expansion coefficients.

"Technique T2" involves the original differential equations (II-4) and (II-5). It involves solving them by perturbation theory without making any Fourier expansions.

In "Technique T3" instead of directly solving the equations for $a(\tau)$ and $b(\tau)$, we focus our attention on the differential equations for the quotients $(a(\tau)/b(\tau))$ and $(b(\tau)/a(\tau))$. We solve for these quotients by a perturbation expansion in the field strength without making any Fourier expansions.

"Technique T4" is just standard steady state perturbation theory.* This is a technique which yields particular solutions for the functions $\eta_a(t)$ and $\eta_b(t)$ in (I-3) under the restriction that $\gamma_a = \gamma_b = 0$. They are particular solutions for the region of t where $t \geq 0$. They arise when, at $t = -\infty$, the two-level system is in either pure stationary state $\psi_a(\underset{\sim}{r})$ or in pure stationary state $\psi_b(\underset{\sim}{r})$ before the $\cos\omega t$ perturbation is adiabatically turned on during the time interval:

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* See Epstein (1969) and Langhoff (1972).

$$-\infty < t < 0 .$$

Convergence of Techniques T1, T2, T3 and T4

All four techniques which we are about to describe converge under the conditions described by (VII-13). The reader who is interested in finding a solution for some regime of the parameters which is included in (VII-13), need only study Technique I since the other techniques include nothing fundamentally different.

Technique T1: Non-Degenerate Rayleigh-Schrödinger Perturbation Theory to Solve (V-3)

In this technique, we will solve the time-independent Schrödinger-type equation, equation (V-3), by making a non-degenerate Rayleigh-Schrödinger expansion in powers of the field strength. Once we have solved the static problem, we may recover the solutions to the dynamic problem of equations (II-4) and (II-5) by utilizing equations (V-7) and (V-8).

H_F is broken up according to (VII-1) and (VII-2) and the expansions (VII-5) and (VII-6) are assumed.

We find that we can obtain one of the Floquet Normal Modes if we choose the zeroth order wavefunction, $|\mu^{(0)}>$, to be

$$|\mu^{(0)}> = |A,j> \qquad \text{(VIII-1)}$$

(our zeroth order energy, $\mu^{(0)}$, is therefore j). We can easily compute the higher-order energies and wavefunctions by the well-known Rayleigh-Schrödinger prescription. By using relationships (V-7) and (V-8) we can use the solution obtained for the static Floquet Hamiltonian to generate a time-dependent Floquet Normal Mode. The final time-dependent result is invariant to the choice of j in (VIII-1).

The other time-dependent Floquet Normal Mode is obtained by letting

$$|\mu^{(0)}> \quad = \quad |B,j> \qquad \text{(VIII-2)}$$

and, therefore

$$\mu^{(0)} \quad = \quad j + \varepsilon - i\delta$$

We now detail the manipulations involved in using non-degenerate Rayleigh-Schrödinger perturbation theory to find the solution of

$$H_F|\mu> \quad = \quad \mu|\mu>$$

which corresponds to choosing

$$\mu^{(0)} \quad = \quad j \quad \text{and} \quad |\mu^{(0)}> \quad = \quad |A,j> \qquad \text{(VIII-3)}$$

where j is any integer or zero. Since H_F, $|\mu>$ and μ are all expanded in powers of λ according to (VII-1), (VII-5), and (VII-6) respectively, we match terms in like powers of λ to obtain a set of solvable equations for the $\mu^{(n)}$'s and $|\mu^{(n)}>$'s .

$$H_F^{(0)}|\mu^{(0)}\rangle = \mu^{(0)}|\mu^{(0)}\rangle \qquad \text{(VIII-4)}$$

$$H_F^{(0)}|\mu^{(1)}\rangle + H_F^{(1)}|\mu^{(0)}\rangle = \mu^{(0)}|\mu^{(1)}\rangle + \mu^{(1)}|\mu^{(0)}\rangle \qquad \text{(VIII-5)}$$

$$H_F^{(0)}|\mu^{(2)}\rangle + H_F^{(1)}|\mu^{(1)}\rangle = \mu^{(0)}|\mu^{(2)}\rangle + \mu^{(1)}|\mu^{(1)}\rangle + \mu^{(2)}|\mu^{(0)}\rangle \,, \quad \text{etc.} \qquad \text{(VIII-6)}$$

The choice of $\mu^{(0)}$ and $|\mu^{(0)}\rangle$ given by (VIII-3) certainly satisfies equation (VIII-4) and, with this choice, the equation for $|\mu^{(1)}\rangle$ becomes:

$$H_F^{(0)}|\mu^{(1)}\rangle + H_F^{(1)}|A,j\rangle = j|\mu^{(1)}\rangle + \mu^{(1)}|A,j\rangle \qquad \text{(VIII-7)}$$

We now solve (VIII-7) by assuming that $|\mu^{(1)}\rangle$ may be expanded in the $|A,k\rangle;|B,k\rangle$ basis:

$$|\mu^{(1)}\rangle = \sum_{k=-\infty}^{\infty} \sum_{\ell=A,B} C_{\ell,k}^{(1)}|\ell,k\rangle \qquad \text{(VIII-8)}$$

where the $C_{\ell,k}^{(1)}$'s are expansion coefficients. If we substitute (VIII-8) into (VIII-7) and left multiply the result by $\langle A,j|$, we find $\mu^{(1)}$:

$$\mu^{(1)} = 0$$

By then left multiplying the result by each and every $<\ell,k|$ we find that all expansion coefficients vanish except $C^{(1)}_{B,j+1}$ and $C^{(1)}_{B,j-1}$. $C^{(1)}_{A,j}$ is not determined by (VIII-7). It is however determined by choosing intermediate normalization of $|\mu>$:

$$<\mu^{(0)}|\mu^{(n)}> \;=\; \delta_{0n}$$

and, with this choice of normalization, $C^{(1)}_{A,j} = 0$. $|\mu^{(1)}>$ therefore is:

$$|\mu^{(1)}> \;=\; \alpha\left[\frac{|B,j-1>}{(1-\varepsilon+i\delta)} - \frac{|B,j+1>}{1+\varepsilon-i\delta}\right] \qquad \text{(VIII-9)}$$

$|\mu^{(2)}>$ is found by solving equation (VIII-6). We again assume that $|\mu^{(2)}>$ may be expanded in the spectrum of $H_F^{(0)}$ and by using the procedure we used to obtain $\mu^{(1)}$ and $|\mu^{(1)}>$, we can find $\mu^{(2)}$ and $|\mu^{(2)}>$. We may, of course, continue this algorithm to obtain results of arbitrary accuracy. The quantities $\mu^{(2)}$ and $|\mu^{(2)}>$ are given in the following summary of results.

$$\mu^{(1)} = 0 = \mu^{(3)} \; ; \quad \mu^{(2)} = \frac{2\alpha^2(\varepsilon - i\delta)}{1 - (\varepsilon - i\delta)^2}$$

$$|\mu^{(1)}\rangle = -\alpha\left[\frac{|B,j+1\rangle}{1+\varepsilon - i\delta} - \frac{|B,j-1\rangle}{1-\varepsilon + i\delta}\right]$$

$$|\mu^{(2)}\rangle = \frac{\alpha^2}{2}\left[\frac{|A,j+2\rangle}{1+\varepsilon - i\delta} + \frac{|A,j-2\rangle}{1-\varepsilon + i\delta}\right] \qquad \text{(VIII-10)}$$

$$+ \alpha\beta\left[\frac{|B,j-2\rangle}{(1-\varepsilon+i\delta)(2-\varepsilon+i\delta)} - \frac{2|B,j\rangle}{1-(\varepsilon-i\delta)^2} + \frac{|B,j+2\rangle}{(1+\varepsilon-i\delta)(2+\varepsilon-i\delta)}\right]$$

From Eq. (VIII-10), by utilizing the correspondence between the eigenvalue-eigenvector problem and the time-dependent problem, we can write a solution to for $a(\tau)$ and $b(\tau)$ which is correct through second order in λ. This solution will be called $a_1(\tau)$ and $b_1(\tau)$ where the subscript "1" is utilized in anticipation of finding another linearly independent solution. This first solution (in which λ has been set equal to unity) is given by:

$$\mu_1 = \frac{2\alpha^2(\varepsilon - i\delta)}{1 - (\varepsilon - i\delta)^2} + \ldots$$

$$a_1(\tau) = e^{-i\mu_1\tau}[1 + \frac{\alpha^2}{2}[\frac{e^{2i\tau}}{1 + \varepsilon - i\delta} + \frac{e^{-2i\tau}}{1 - \varepsilon + i\delta}] + \ldots]$$

$$b_1(\tau) = e^{-i\mu_1\tau}\phi_{b1}(\tau)$$

$$\phi_{b1}(\tau) = \alpha[\frac{e^{-i\tau}}{1 - \varepsilon + i\delta} - \frac{e^{i\tau}}{1 + \varepsilon - i\delta}] + \alpha\beta\left[\frac{e^{2i\tau}}{(1 + \varepsilon - i\delta)(2 + \varepsilon - i\delta)} - \frac{2}{1 - (\varepsilon - i\delta)^2} + \frac{e^{-2i\tau}}{(1 - \varepsilon + i\delta)(2 - \varepsilon + i\delta)}\right] + \ldots. \tag{VIII-11}$$

Letting $|\mu^{(0)}\rangle = |B,j\rangle$ and $\mu^{(0)} = j + \varepsilon - i\delta$, we can obtain the other Floquet Normal Mode which we will call $\{a_2(\tau),b_2(\tau)\}$. It is correct through second order in λ and it is given by:

$$\mu_2 = \varepsilon - i\delta - \frac{2\alpha^2(\varepsilon - i\delta)}{1 - (\varepsilon - i\delta)^2} + \ldots$$

$$a_2(\tau) = e^{-i\mu_2\tau}\left[\alpha(\frac{e^{-i\tau}}{1 + \varepsilon - i\delta} - \frac{e^{i\tau}}{1 - \varepsilon + i\delta}) + \alpha\beta(\frac{e^{-2i\tau}}{2 + \varepsilon - i\delta} + \frac{e^{2i\tau}}{2 - \varepsilon + i\delta}) + \ldots\right]$$

$$b_2(\tau) = e^{-i\mu_2\tau}\left[1 + \beta(e^{-i\tau} - e^{i\tau}) + \frac{\beta^2}{2}(e^{-2i\tau} + e^{2i\tau}) + \frac{\alpha^2}{2}(\frac{e^{-2i\tau}}{1 + \varepsilon - i\delta} + \frac{e^{2i\tau}}{1 - \varepsilon + i\delta}) + \ldots\right] \tag{VIII-12}$$

From (VIII-11) and VIII-12), we can empirically confirm the convergence conditions we postulated in (VII-10). We can also check the algebra involved in deriving our results by using the relationship between any two linearly independent solutions which is given by (III-21). Further, since the solutions are either Form I or Form II, we may express the general solution which satisfies arbitrary initial conditions in terms of (VIII-11) and (VIII-12):

$$a(\tau) = C_1 a_1(\tau) + C_2 a_2(\tau)$$

$$b(\tau) = C_1 b_1(\tau) + C_2 b_2(\tau)$$

where C_1 and C_2 are arbitrary constants.

Sen Gupta's Technique: Technique T2

The next approach to be considered (call it "Technique T2") was used by Sen Gupta (1970). It involves directly solving the differential equations, (II-4) and (II-5), without first making a Fourier Expansion.

The first step in the approach is to assume that the solution is of the Floquet form:

$$\begin{aligned} a(\tau) &= e^{-i\mu\tau}\phi_a(\tau) \\ b(\tau) &= e^{-i\mu\tau}\phi_b(\tau) \end{aligned} \qquad \text{(VIII-13)}$$

We do not make a Fourier Expansion of ϕ_a and ϕ_b but rather substitute (VIII-13) into (II-4) and (II-5) to obtain equations for the ϕ's .

$$\begin{aligned} \dot{\phi}_a &= i\mu\phi_a - 2i\alpha\cos\tau\phi_b \\ \dot{\phi}_b &= i\mu\phi_b - i(\varepsilon - i\delta)\phi_b - 2i\beta\cos\tau\phi_b - 2i\alpha\cos\tau\phi_a \end{aligned} \tag{VIII-14}$$

We will consider α and β to be the perturbations in (VIII-14). We may formally do this by introducing the ordering parameter λ which will be set equal to unity whenever final results are reported. With the introduction of λ , (VIII-14) becomes:*

$$\begin{aligned} \dot{\phi}_a &= i\mu\phi_a - 2i\lambda\alpha\cos\tau\phi_b \\ \dot{\phi}_b &= i\mu\phi_b - i(\varepsilon - i\delta)\phi_b - 2i\lambda\beta\cos\tau\phi_b - 2i\alpha\lambda\cos\tau\phi_a \end{aligned} \tag{VIII-15}$$

We next assume that ϕ_a, ϕ_b and the characteristic exponent, μ , may be expanded in a power series in λ :

$$\mu = \sum_{n=0}^{\infty} \lambda^n \mu^{(n)} \; ; \quad \phi_k(\tau) = \sum_{n=0}^{\infty} \lambda^n \phi_k^{(n)}(\tau) \qquad k = a,b \tag{VIII-16}$$

---

* Note that the introduction of λ in this manner is equivalent to an expansion in the field strength, F .

Substituting the expansions (VIII-16) into (VIII-15) and grouping together terms in similar powers of λ , we can obtain solvable equations for $\mu^{(n)}$ and $\phi_k^{(n)}$ $(k = a,b)$. In solving these equations, the $\mu^{(n)}$'s are determined by requiring that the $\phi_k^{(n)}$'s have the proper periodicity, i.e.

$$\phi_k^{(n)}(\tau) = \phi_k^{(n)}(\tau + 2\pi) \; ; \quad k = a,b; \text{ all } n . \tag{VIII-17}$$

For example, the zeroth order equations are:

$$\begin{aligned} \dot{\phi}_a^{(0)} &= i\mu^{(0)} \phi_a^{(0)} \\ \dot{\phi}_b^{(0)} &= i\mu^{(0)} \phi_b^{(0)} - i(\varepsilon - i\delta)\phi_b^{(0)} \end{aligned} \tag{VIII-18}$$

(VIII-18) are uncoupled and therefore may be immediately solved to give

$$\phi_a^{(0)} = K_a^{(0)} e^{i\mu^{(0)}\tau}$$

$$\phi_b^{(0)} = K_b^{(0)} e^{i[\mu^{(0)}-\varepsilon+i\delta]\tau}$$

where $K_a^{(0)}$ and $K_b^{(0)}$ are constants of integration.

We must now choose the constants $\mu^{(0)}$, $K_a^{(0)}$ and $K_b^{(0)}$ so that condition (VIII-17) is obeyed. If ε is <u>non-integer</u>, this may be accomplished in two ways:

<u>Choice I</u>: $\mu^{(0)} = m$; $K_b^{(0)} = 0$; $K_a^{(0)}$ arbitrary

<u>Choice II</u>: $\mu^{(0)} = m + \varepsilon - i\delta$; $K_a^{(0)} = 0$; $K_b^{(0)}$ arbitrary

where m is any (positive or negative) integer or zero. When ε is <u>non-integer</u>, choosing the constants of integration is a simple matter since any term which involves an arbitrary constant times an $\exp[\pm i\varepsilon\tau]$ factor can only be properly periodic if the arbitrary constant is set equal to zero. When $\delta = 0$ and ε is integer, slight complications arise which we can ignore, since, when ε is exactly or almost equal to an integer, we recommend that entirely different perturbation techniques be used (see Chapters XI and XII). If we start with Choice I and carry out the calculation to higher orders, we find that the $\mu^{(n)}$'s are determined in each and every order by the requirement (VIII-17). Furthermore starting with Choice I, we are led to exactly the same result as the result given by (VIII-11), i.e. we are led to one of the Floquet Normal Modes. Starting with Choice II, we end up with the other Floquet Normal Mode, i.e. exactly the expression in equation (VIII-12).

<u>Manipulations Involved in T2</u>.

To accomplish the task of explaining Technique T2, we only need to follow the development arising from Choice I since the manipulations arising from Choice II are similar. We will also find that the results are exactly same no matter what we choose m to be. If, for simplicity, we let $m = 0$ and let $K_a^{(0)} = 1$ we have the Choice I-zeroth order solution:

$$\mu^{(0)} = 0 \; ; \quad \phi_a^{(0)} = 1 \; ; \quad \phi_b^{(0)} = 0 \qquad \text{(VIII-19)}$$

Using (VIII-19) in the perturbation equations proportional to λ we have

$$\dot{\phi}_a^{(1)} = i\mu^{(1)} \qquad \text{(VIII-20)}$$

$$\dot{\phi}_b^{(1)} = -i(\varepsilon - i\delta)\phi_b^{(1)} - 2i\alpha\cos\tau \qquad \text{(VIII-21)}$$

These first order equations may be easily solved* to obtain:

$$\phi_a^{(1)} = K_a^{(1)} + i\mu^{(1)}\tau$$

$$\phi_b^{(1)} = K_b^{(1)} \exp[-i(\varepsilon - i\delta)\tau] + \alpha\left[\frac{e^{-i\tau}}{1 - \varepsilon + i\delta} - \frac{e^{i\tau}}{1 + \varepsilon - i\delta}\right]$$

where $K_a^{(1)}$ and $K_b^{(1)}$ are constants of integration. $\phi_a^{(1)}$ is periodic <u>only if</u> we choose $\mu^{(1)} = 0$. This manner of determining the $\mu^{(n)}$'s is a hallmark of this technique, namely: the $\mu^{(n)}$'s are chosen so that they cancel out terms linear in τ which appear in the $\phi_j^{(n)}$'s . To use an older phraseology, the $\mu^{(n)}$'s are chosen to make the secular terms in the $\phi_j^{(n)}$'s vanish and thereby make the $\phi_j^{(n)}$'s have the proper periodicity.

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* The equation for $\phi_b^{(1)}$ is a standard equation--the solution of which is given by Dwight (1961) on page 252.

If ε is non-integer, $\phi_b^{(1)}$ is periodic if and only if $K_b^{(1)} = 0$ and therefore the periodicity requirement determines the constant of integration.

Choosing* $K_a^{(1)} = 0$, we summarize the first order results:

$$\mu_b^{(1)} = 0 \; ; \quad \phi_a^{(1)} = 0$$

$$\phi_b^{(1)} = \alpha\left[\frac{e^{-i\tau}}{1 - \varepsilon + i\delta} - \frac{e^{i\tau}}{1 + \varepsilon - i\delta}\right] \tag{VIII-22}$$

With the zeroth and first order results established, we write the equations proportional to λ^2 :

$$\dot{\phi}_a^{(2)} = i\mu^{(2)} - 2i\alpha\cos\tau\, \phi_b^{(1)}$$

$$\dot{\phi}_b^{(2)} = -i(\varepsilon - i\delta)\phi_b^{(2)} - 2i\beta\cos\tau\, \phi_b^{(1)} - 2i\alpha\cos\tau\, \phi_a^{(1)}$$

These equations are easily solved to obtain expressions for $\phi_a^{(2)}$ and $\phi_b^{(2)}$ which involve the constants of integration $K_a^{(2)}$ and $K_b^{(2)}$:

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* We are free to choose $K_a^{(1)}$ to be anything we want. This corresponds to choosing normalization.

$$\phi_a^{(2)} = K_a^{(2)} + i\mu^{(2)}\tau + \frac{i\alpha^2}{2}\left[\frac{(2\tau - ie^{2i\tau})}{(1 + \varepsilon - i\delta)} - \frac{(2\tau + ie^{-2i\tau})}{(1 - \varepsilon + i\delta)}\right]$$

$$\phi_b^{(2)} = K_b^{(2)} \exp[-i(\varepsilon-i\delta)\tau] + \alpha\beta\left[\frac{e^{2i\tau}}{(1+\varepsilon-i\delta)(2+\varepsilon-i\delta)} + \frac{e^{-2i\tau}}{(1-\varepsilon+i\delta)(2-\varepsilon+i\delta)} - \frac{2}{[1-(\varepsilon-i\delta)^2]}\right]$$

(VIII-23)

In Eq. (VIII-23), $\phi_a^{(2)}$ is made periodic by choosing $\mu^{(2)}$ so that it cancels out the terms linear in τ. For $\phi_b^{(2)}$ to be periodic, we must set $K_b^{(2)}$ equal to zero. Therefore, we let

$$K_b^{(2)} = 0 \quad \text{and} \quad \mu^{(2)} = \frac{2\alpha^2(\varepsilon-i\delta)}{1-(\varepsilon-i\delta)^2}$$

We can continue this procedure to obtain even higher order corrections. We would find that all $K_b^{(n)}$'s and all $\mu^{(n)}$'s would be uniquely determined by the periodicity requirements on the $\phi_j^{(n)}$'s. The $K_a^{(n)}$'s are arbitrary and are chosen to fit whatever normalization requirements we might impose. If we specify $K_a^{(0)} = 1$ and $K_a^{(n)} = 0$ $(n > 0)$, the solution we obtain is exactly the Floquet solution given by (VIII-11).

Similarly if we use this perturbation scheme starting off with Choice II, we will get exactly the Floquet solution given by (VIII-12) if we choose the normalization:

$$K_b^{(0)} = 1 \; ; \quad K_b^{(n)} = 0 \quad (n > 0)$$

The fact that this technique leads to solutions exactly equivalent to the non-degenerate Rayleigh-Schrödinger results, means that this technique will give solutions which are quickly convergent only under the conditions given in (VII-13). This observation should make us stop and think before we apply techniques such as "Technique II" in solving systems such as (VIII-15). With this technique, in zeroth order we are neglecting only terms proportional to λ (i.e. proportional to the field strength). We are retaining the terms $\dot{\phi}_a$, $\dot{\phi}_b$ and $-i(\varepsilon - i\delta)\phi_b$. We might, at first sight, expect the perturbation solutions obtained to converge for large ε and large δ . They will not converge, of course, in the case of arbitrary large ε , because by (VII-13), if $\varepsilon \approx n$ (n any integer) and δ is very small, the solutions would not be quickly convergent.

The Technique T1 formulation of the original time-dependent problem as a static problem therefore has an advantage over the Technique T2 formulation. Because of our familiarity with the static problem and its convergence properties, Technique T1 gives us a set of convergence requirements which are not as easily seen in techniques such as T2 which do not directly involve the Fourier Expansion.

Technique T3: Field Strength Perturbations Of the Quotient Equations

The approach which we are calling "Technique T3" starts off by considering the differential equations for the quotients $b(\tau)/a(\tau)$ and $a(\tau)/b(\tau)$. In it, no Fourier Expansions are made. The resulting equations, however, are solved by a perturbation expansion in the field strength, F .

Block and Siegert (1940) used these quotient equations in considering the effect of the field strength on the resonance frequency. Their method of solution, however, is very different from the technique we are about to describe. The Langhoff-Epstein-Karplus (1972) time-dependent steady state perturbation formalism, when applied to the two-level system with $\gamma_a = \gamma_b = 0$, essentially reduces to solving the quotient equations by making a perturbation expansion in the field strength, F .

In Technique T3, we start off by letting

$$b_1(\tau)/a_1(\tau) = \Phi_1(\tau) \tag{VIII-24}$$

For the case of $\{a_1(\tau), b_1(\tau)\}$ being one of the Floquet Normal Mode particular solutions,

$$\Phi_1(\tau + 2\pi) = \Phi_1(\tau) .$$

Using (II-4) and (II-5), we may find the differential equation which Φ_1 obeys. It is:

$$\dot{\Phi}_1 = -i(\varepsilon - i\delta + 2\beta\cos\tau)\Phi_1 - 2i\alpha\cos\tau + 2i\alpha\cos\tau(\Phi_1)^2 \quad \text{(VIII-25)}$$

Note that the equation for Φ_1 is a first order non-linear equation. Once Φ_1 is known, however, we can recover $a_1(\tau)$ and $b_1(\tau)$, since by using the definition of Φ_1 in equation (II-4), we have:

$$\dot{a}_1 = -2i\alpha\cos\tau\Phi_1 a_1$$

therefore

$$a_1 = K_a \exp[\int(-2i\alpha\cos\tau\Phi_1(\tau)d\tau]$$

where K_a is a constant of integration. If we define $\theta_1(\tau)$ by,

$$\dot{\theta}_1 = -2i\alpha\cos\tau\Phi_1(\tau) \quad \text{(VIII-26)}$$

then we may write the solution to (II-4) and (II-5) as

$$a_1(\tau) = \exp[\theta_1(\tau)]$$
$$b_1(\tau) = \Phi_1(\tau)\exp[\theta_1(\tau)] \qquad \text{(VIII-27)}$$

Solving equations (VIII-25) and (VIII-26) is equivalent to solving (II-4) and (II-5).

In the same manner, we can look at the quotient

$$a_2(\tau)/b_2(\tau) = \Phi_2(\tau) \qquad \text{(VIII-28)}$$

The equation for $\Phi_2(\tau)$ is first order and non-linear:

$$\dot{\Phi}_2 = -2i\alpha\cos\tau + i(\varepsilon - i\delta + 2\beta\cos\tau)\Phi_2 + 2i\alpha\cos\tau(\Phi_2)^2 \qquad \text{(VIII-29)}$$

Once we know $\Phi_2(\tau)$, we can recover $a_2(\tau)$ and $b_2(\tau)$ by substituting $a_2(\tau) = \Phi_2(\tau)b_2(\tau)$ into (II-5). If we define $\theta_2(\tau)$ by*

$$\dot{\theta}_2 = -i(\varepsilon - i\delta + 2\beta\cos\tau) - 2i\alpha\cos\tau\Phi_2(\tau) \qquad \text{(VIII-30)}$$

then we may write the solution to (II-4) and (II-5) as

---

* Note that if $\Phi_2(\tau)$ is known, $\theta_2(\tau)$ may be found by simple quadrature.

$$a_2(\tau) = \Phi_2(\tau)\exp[\theta_2(\tau)]$$
$$b_2(\tau) = \exp[\theta_2(\tau)] \qquad \text{(VIII-31)}$$

Equations (VIII-29) and (VIII-30) are therefore also equivalent to equations (II-4) and (II-5).

What we now want to do, is to solve the non-linear equations, (VIII-25) and (VIII-30), by an expansion in the field strength to obtain the Floquet Normal Modes. We will find that solution of (VIII-25) will yield one Floquet Normal Mode and that solution of (VIII-30) will yield the other one.

Let us first focus on (VIII-25). If we assume that

$$a_1(\tau) = e^{-i\mu\tau}\phi_a(\tau) \ ; \quad b_1(\tau) = e^{-i\mu\tau}\phi_b(\tau)$$

where μ is a constant and $\phi_k(\tau) = \phi_k(\tau + 2\pi)$ $(k = a,b)$, then it follows that

$$\Phi_1(\tau) = \Phi_1(\tau + 2\pi) \qquad \text{(VIII-32)}$$

Therefore, to obtain a Floquet Normal Mode particular solution, we must impose condition (VIII-32) on Φ_1.

We can obtain a perturbation solution for Φ_1 in powers of the field strength. We do this by introducing the ordering parameter λ and by replacing α and β wherever they appear in (VIII-25) by $\lambda\alpha$ and $\lambda\beta$ respectively:

$$\dot{\Phi}_1 = -i(\epsilon-i\delta)\Phi_1 - 2i\lambda\beta\cos\tau\Phi_1 - 2i\lambda\alpha\cos\tau + 2i\lambda\alpha\cos\tau(\Phi_1)^2 \quad \text{(VIII-33)}$$

We assume the following expansion for Φ_1 :

$$\Phi_1(\tau) = \sum_{n=0}^{\infty} \lambda^n \Phi_1^{(n)}(\tau) \quad \text{(VIII-34)}$$

Substituting this expansion into Eq. (VIII-33), we match like powers of the ordering parameter λ to obtain a set of solvable perturbation equations the first three of which are:

$$\dot{\Phi}_1^{(0)} = -i(\epsilon-i\delta)\Phi_1^{(0)} \quad \text{(VIII-35)}$$

$$\dot{\Phi}_1^{(1)} = -i(\epsilon-i\delta)\Phi_1^{(1)} - 2i\beta\cos\tau\Phi_1^{(0)} + 2i\alpha\cos\tau[\Phi_1^{(0)}]^2 - 2i\alpha\cos\tau \quad \text{(VIII-36)}$$

$$\dot{\Phi}_1^{(2)} = -i(\epsilon-i\delta)\Phi_1^{(2)} - 2i\beta\cos\tau\Phi_1^{(1)} + 4i\alpha\cos\tau\Phi_1^{(1)}\,\Phi_1^{(0)} \quad \text{(VIII-37)}$$

Since we have defined Φ_1 by

$$\Phi_1(\tau) = b_1(\tau)/a_1(\tau) ,$$

if we are seeking a Floquet particular solution we must require

$$\Phi_1(\tau+2\pi) = \Phi_1(\tau)$$

In terms of the λ-expansion of Φ_1 , this requirement becomes:

$$\Phi_1^{(n)}(\tau+2\pi) = \Phi_1^{(n)}(\tau) \qquad \text{all } n . \qquad \text{(VIII-38)}$$

The solution to (VIII-35) is

$$\Phi_1^{(0)} = K_1^{(0)} \exp[-i(\varepsilon-i\delta)\tau]$$

If ε is non-integer,* the only way in which (VIII-38) can be fulfilled is by requiring $K_1^{(0)} = 0$. Stipulating that ε be non-integer we therefore have:

$$\Phi_1^{(0)} = 0 \qquad \text{(VIII-39)}$$

We now solve equation (VIII-36) which becomes with $\Phi_1^{(0)} = 0$:

$$\dot{\Phi}_1^{(1)} = -i(\varepsilon-i\delta)\Phi_1^{(1)} - 2i\alpha\cos\tau$$

Letting $K_1^{(1)}$ be the constant of integration, we write the solution for $\Phi_1^{(1)}$:

---

* If $\delta = 0$ and ε is integer, $K_1^{(0)}$ is not determined by the zero-order periodicity requirement. It will be determined in some higher order of the perturbation. We can ignore this complication, since, when ε is integer we recommend that entirely different techniques of solution be used.

$$\Phi_1^{(1)} = \alpha\left[\frac{e^{-i\tau}}{1-\varepsilon+i\delta} - \frac{e^{i\tau}}{1+\varepsilon-i\delta}\right] + K_1^{(1)} e^{-i(\varepsilon-i\delta)\tau}$$

Since ε is non-integer, the constant of integration, $K_1^{(1)}$, must be set equal to zero if $\Phi_1^{(1)}$ is to obey (VIII-38). We use $\Phi_1^{(1)}$ in (VIII-37) and obtain the equation for $\Phi_1^{(2)}$. In solving this equation, we again find that proper periodicity requires that the constant of integration appearing in it be set equal to zero. $\Phi_1^{(2)}$ is found to be:

$$\Phi_1^{(2)} = \alpha\beta\left[\frac{e^{2i\tau}}{(1+\varepsilon-i\delta)(2+\varepsilon-i\delta)} - \frac{2}{1-(\varepsilon-i\delta)^2} + \frac{e^{-2i\tau}}{(1-\varepsilon+i\delta)(2-\varepsilon+i\delta)}\right] \tag{VIII-39}$$

This development may easily be carried on to obtain the higher order terms in Φ_1. We may also use exactly the same techniques to find a periodic solution to (VIII-29).

Since we have an approximation to Φ_1, we now obtain an approximation to θ_1 by using (VIII-26). In doing this we must resolve the question of normalization. In order to easily compare our present results to the Technique T1 solutions we impose the following normalization condition:

$$\exp[\theta_1(\tau=0)] = 1 + \frac{\lambda^2\alpha^2}{1-(\varepsilon-i\delta)^2} \tag{VIII-40}$$

To apply this condition, we will first assume that θ_1 may be expanded in a power series in λ :

$$\theta_1 = \theta_1^{(0)} + \lambda\theta_1^{(1)} + \lambda^2\theta_1^{(2)} + \ldots \qquad \text{(VIII-41)}$$

If this expansion is substituted into (VIII-40) and if the exponential is expanded according to:

$$e^{\theta_1} = e^{\theta_1^{(0)}}[1 + \lambda\theta_1^{(1)} + \lambda^2(\theta_1^{(2)} + \tfrac{1}{2}[\theta_1^{(1)}]^2) + \ldots]$$

we now match like powers of λ and set $\tau = 0$ to obtain:

$$\theta_1^{(0)}(0) = 0 \; ; \quad \theta_1^{(1)}(0) = 0 \; ; \quad \theta_1^{(2)}(0) = \frac{\alpha^2}{1-(\varepsilon-i\delta)^2} \qquad \text{(VIII-42)}$$

In solving (VIII-26), we first replace α by $(\lambda\alpha)$. Inserting the λ-expansions of θ_1 and Φ_1 , we obtain the equations proportional to λ^0 and λ :

$$\dot{\theta}_1^{(0)} = 0 \; ; \quad \dot{\theta}_1^{(1)} = 0$$

Both $\theta_1^{(0)}$ and $\theta_1^{(1)}$ are therefore constants, and by the normalization in (VIII-42) both of these constants must be zero. From the equation proportional to λ^2 we have:

$$\dot{\theta}_1^{(2)} = -2i\alpha\cos\tau\Phi_1^{(1)}$$

Its solution is simply:

$$\theta_1^{(2)} = K_\theta^{(2)} - \frac{2i\alpha^2(\varepsilon-i\delta)\tau}{1-(\varepsilon-i\delta)^2} + \frac{\alpha^2}{2}\left[\frac{e^{-2i\tau}}{1-\varepsilon+i\delta} + \frac{e^{2i\tau}}{1+\varepsilon-i\delta}\right]$$

$K_\theta^{(2)}$ may be found from the normalization conditions given by (VIII-42):

$$K_\theta^{(2)} \doteq 0$$

Since we know $\Phi_1^{(2)}$, we could continue this process to find $\theta_1^{(3)}$. Since nothing illustrative is gained by doing so, we will just report the results giving θ_1 correct through λ^2.

All of these results for $\Phi_1(\tau)$ and $\theta_1(\tau)$ are now used in Eq. (VIII-27) to obtain expressions for $\{a_1(\tau);b_1(\tau)$. We get a Floquet particular solution which is correct through second order in λ, and, in which, λ has been set equal to unity:

$$a_1(\tau) = \exp[\theta_1(\tau)] \; ; \qquad b_1(\tau) = \Phi_1(\tau)\exp[\theta_1(\tau)]$$

$$\theta_1 = \frac{-2i\alpha^2(\varepsilon-i\delta)\tau}{1-(\varepsilon-i\delta)^2} + \frac{\alpha^2}{2}\left[\frac{e^{2i\tau}}{1+\varepsilon-i\delta} + \frac{e^{-2i\tau}}{1-\varepsilon+i\delta}\right] + \ldots$$

$$\Phi_1(\tau) = \alpha\left[\frac{e^{-i\tau}}{1-\varepsilon+i\delta} - \frac{e^{i\tau}}{1+\varepsilon-i\delta}\right] + \alpha\beta\left[\frac{e^{2i\tau}}{(1+\varepsilon-i\delta)(2+\varepsilon-i\delta)} - \frac{2}{1-(\varepsilon-i\delta)^2} + \frac{e^{-2i\tau}}{(1-\varepsilon+i\delta)(2-\varepsilon+i\delta)}\right] + \ldots.$$

(VIII-43)

The normalization given by (VIII-40) has been chosen to facilitate the comparison of the results in (VIII-43) with the previous results given by (VIII-11).

Notice that secular terms (terms linear in τ) appear only in θ_1 . If we write (VIII-43) in terms of the independent variable $t = \tau/\omega$ and let $\varepsilon = \Delta W/\omega$, $\alpha = FVab/\omega$, etc., we find that terms in inverse powers of ω appear only in θ_1 . This is in accord with what Epstein (1969) and Langhoff (1972) predict for solutions which have been written as (VIII-27) and (VIII-31).

Note the curious fact that the field stength perturbation expansion of (VIII-25) yields only one of the Floquet Normal Modes in spite of the fact that all solutions $b(\tau)/a(\tau)$ obey (VIII-25). To obtain the other Floquet Mode, we must perturbatively solve (VIII-29) using a field strength expansion.

Proceeding in the same manner as we did in deriving the first Floquet Mode (equation (VIII-43)), we can derive the other Floquet Normal Mode. It is given by the following expression which is correct through λ^2 and, in which, λ has been set equal to unity.

$$a_2 = \Phi_2(\tau)\exp[\theta_2(\tau)] \; ; \quad b_2 = \exp[\theta_2(\tau)]$$

$$\theta_2(\tau) = -(i\varepsilon + \delta)\tau + \beta(e^{-i\tau} - e^{i\tau}) + \beta^2 + \frac{2i\alpha^2(\varepsilon - i\delta)\tau}{1 - (\varepsilon - i\delta)^2}$$
$$+ \frac{\alpha^2}{2}\left[\frac{e^{-2i\tau}}{(1 + \varepsilon - i\delta)} + \frac{e^{2i\tau}}{(1 - \varepsilon + i\delta)}\right] + \ldots$$

(VIII-44)

$$\Phi_2(\tau) = \alpha\left[\frac{e^{-i\tau}}{1 + \varepsilon - i\delta} - \frac{e^{i\tau}}{1 - \varepsilon + i\delta}\right]$$
$$+ \alpha\beta\left[\frac{2}{1 - (\varepsilon - i\delta)^2} - \frac{e^{-2i\tau}}{(2 + \varepsilon - i\delta)(1 + \varepsilon - i\delta)} - \frac{e^{2i\tau}}{(2 - \varepsilon + i\delta)(1 - \varepsilon + i\delta)}\right] + \ldots.$$

We have normalized (VIII-44) according to

$$\exp[\theta_2(0)] = 1 + \beta^2 + \frac{\alpha^2}{1 - (\varepsilon - i\delta)^2} + \ldots.$$

Mere inspection of (VIII-43) and (VIII-44) would lead us to postulate that they will only converge under the same requirements we imposed for Technique I solutions to converge. This postulate is further confirmed when we realize that (VIII-11) can be obtained from (VIII-43) and (VIII-5) can be obtained from (VIII-44). For example the equivalence of (VIII-43) to the solution given by (VIII-11) can be established by taking (VIII-43) and expanding those terms in the exponent of a_1 and b_1 not linear in τ . In detail, we can do this by separating θ_1 into

$$\theta_1(\tau) \;=\; \bar{\theta}_1(\tau) + \hat{\theta}_1(\tau)$$

$\bar{\theta}_1$ contains only the terms linear in τ and $\hat{\theta}_1$, contains all other terms. Now expand $\exp(\theta_1)$ according to (VIII-45)

$$\exp[\theta_1] \;=\; \exp[\bar{\theta}_1 + \hat{\theta}_1] \;=\; [1 + \hat{\theta} + \frac{(\hat{\theta})^2}{2!} + \ldots]\exp[\bar{\theta}_1] \qquad \text{(VIII-45)}$$

If we use (VIII-45) in (VIII-43), replace α by $\lambda\alpha$ and β by $\lambda\beta$, we find after regrouping like powers of λ that we have recovered the solution given in (VIII-11) after we have discarded terms going as λ^n where $n \geq 3$ and have set λ equal to unity.

We can generate (VIII-12) from (VIII-44) in exactly the same manner.

The Technique T3 Solutions for η_a and η_b When $\gamma_a = \gamma_b = \delta = 0$

We wish to write down the Technique III solutions for η_a and η_b when $\gamma_a = \gamma_b = \delta = 0$. We will need these in subsequent sections of the report when we discuss the steady-state perturbation theory.

Recall that $\{\eta_a(t),\eta_b(t)\}$ is related to $\{a(\tau),b(\tau)\}$ by (II-1) and (II-2) and the reduced parameters are related to the non-reduced parameters by (II-3). The Floquet Normal Modes Solutions given by (VIII-43) and (VIII-44) for the case of $\gamma_a = \gamma_b = 0$ give the following solutions for $\eta_a(t)$ and $\eta_b(t)$.

The Floquet Normal Mode which has been obtained from (VIII-43) may be written as:

$$\eta_{a1} = \exp[\theta_1'(t)] \; ; \quad \eta_{b1} = \Phi_1'(t)\exp[\theta_1'(t)]$$

$$\theta_1'(t) = -iW_a t - 2i\frac{FV_{aa}}{\omega}\sin\omega t - \frac{2i(FV_{ab})^2\Delta Wt}{\omega^2 - (\Delta W)^2} + \frac{(FV_{ab})^2}{2\omega}\left[\frac{e^{2i\omega t}}{\omega + \Delta W} + \frac{e^{-2i\omega t}}{\omega - \Delta W}\right] \qquad \text{(VIII-46)}$$

$$\Phi_1'(t) = FV_{ab}\left[\frac{e^{-i\omega t}}{\omega - \Delta W} - \frac{e^{i\omega t}}{\omega + \Delta W}\right] + F^2V_{ab}\Delta V\left[\frac{e^{2i\omega t}}{(\omega + \Delta W)(2\omega + \Delta W)} - \frac{2}{\omega^2 - (\Delta W)^2} + \frac{e^{-2i\omega t}}{(\omega - \Delta W)(2\omega - \Delta W)}\right]$$

where $\Delta W = W_b - W_a$ and $\Delta V = V_{bb} - V_{aa}$.

The other Floquet Normal Mode is obtained from (VIII-44) and it is:

$$\eta_{a2} = \Phi_2'(t)\exp[\theta_2'(t)] \; ; \quad \eta_{b2} = \exp[\theta_2'(t)]$$

$$\theta_2'(t) = -iW_b t - \frac{2iFV_{bb}}{\omega}\sin\omega t + (F^2\Delta V)^2 + \frac{2i(FV_{ab})^2\Delta Wt}{\omega^2 - (\Delta W)^2} + \frac{(FV_{ab})^2}{2\omega}\left[\frac{e^{-2i\omega t}}{\omega + \Delta W} + \frac{e^{2i\omega t}}{\omega - \Delta W}\right] \qquad \text{(VIII-47)}$$

$$\Phi_2'(t) = FV_{ab}\left[\frac{e^{-i\omega t}}{\omega + \Delta W} - \frac{e^{i\omega t}}{\omega - \Delta W}\right] + F^2V_{ab}\Delta V\left[\frac{2}{\omega^2 + (\Delta W)^2} - \frac{e^{-2i\omega t}}{(2\omega + \Delta W)(\omega + \Delta W)} - \frac{e^{2i\omega t}}{(2\omega - \Delta W)(\omega - \Delta W)}\right]$$

Inspection of (VIII-46) and (VIII-47) as well as consideration of the convergence criteria given by (VII-13), leads us to postulate that the expressions (VIII-46) and (VIII-47) for the Floquet Normal Modes will be quickly convergent under the following conditions:

$\frac{FV_{ab}}{\omega}$, $\frac{FV_{aa}}{\omega}$ and $\frac{FV_{bb}}{\omega}$ are all much less than unity
and these quantities are all much less than
$\left|\frac{\Delta W}{\omega} - K_{min}\right|$ where K_{min} is the integer which makes
$\left|\frac{\Delta W}{\omega} - K_{min}\right|$ as small as possible. (VIII-48)

The one point which we wish to stress (and we will come back to this point when we discuss steady-state perturbation theory) is that we do not expect expressions (VIII-46) and (VIII-47) to be convergent expressions whenever $\Delta W/\omega$ is almost equal or exactly equal to some non-zero integer. In fact, if $\Delta W/\omega = n$ (n some non-zero integer) we would expect that the n-th order correction to Φ_1' and Φ_2' would to be infinitely large. This is so because we expect to have a denominator of the form

$$(n\omega - \Delta W)$$

in the n-th order of perturbation.

Technique T4: Steady-State Perturbation Theory

The last remaining field-strength expansion technique which we wish to discuss is the "Steady-State Time-Dependent Perturbation Theory." This technique is very fully discussed in Epstein's (1969) report and in the 1972 review article written by Langhoff, Epstein and Karplus.

The steady-state perturbation theory is meant to apply to the original equations for $\eta_a(t)$ and $\eta_b(t)$ (equations (I-4) and (I-5)) under the conditions that $\gamma_a = \gamma_b = 0$. The theory gives us the appropriate particular solution for

$$\Psi(\underset{\sim}{r},t) \;=\; \eta_a(t)\psi_a(\underset{\sim}{r}) + \eta_b(t)\psi_b(\underset{\sim}{r})$$

in the regime of time, $t \geq 0$, when at $t = -\infty$ the two-level system is in the pure quantum state $\psi_k(\underset{\sim}{r})$ (k = a or b) and the $\cos\omega t$ perturbation is adiabatically turned on. These "steady-state" solutions are the particular solutions used in the computation of the optical properties of matter such as the index of refraction, etc.

We use our simple two-level model problem to demonstrate two points.

The first point we show is that these steady-state solutions are just the Floquet Normal Mode particular solutions. If at $t = -\infty$, the two-level system is in quantum state $\psi_a(\underset{\sim}{r})$ and if the $\cos\omega t$ perturbation is adiabatically turned on, in the regime of $t \geq 0$, the system will be in one of the Floquet Normal Modes. The system will be in the other Floqet Normal Mode, if before the $\cos\omega t$ perturbation is adiabatically turned on, the system is in pure stationary state $\psi_b(\underset{\sim}{r})$. The equivalence between the steady-state solutions and the Floquet Normal Modes has been discussed in the recent literature. Young, Deal and Kestner (1969) call the Floquet particular solutions "quasi-periodic states" and assert that these quasi-periodic solutions are the steady-state solutions. Sambe (1973) and Okuniewicz (1972) discuss how, after one has made the correspondence between the Floquet solutions and the steady-state solutions, one may treat the problem of a quantum system in a periodic perturbation by borrowing some of the techniques used in time-independent quantum theory. In their treatment of the high-frequency Stark Effect, Hicks, Hess and Cooper (1972) seek the steady-state solutions for a periodically perturbed system by seeking the Floquet Modes of the system. Young and Deal (1970) prove that an adiabatically turned-on periodic perturbations will put a quantum system in a Floquet Normal Mode.

The other point we show is that the Langhoff-Epstein-Karplus formalism yields expressions for the Floquet Normal Modes which (aside from phase and normalization) are exactly equivalent to the expressions for the Floquet Modes which we would obtain if we applied Technique T3 to the equations for $\eta_a(t)$ and $\eta_b(t)$ and let $\gamma_a = \gamma_b = 0$, i.e. expressions (VIII-46) and (VIII-47).

We discuss and demonstrate the two points we have just mode after we restate the formalism described by Langhoff, Epstein, and Karplus (1972).

Restatement of the Langhoff-Epstein-Karplus Formalism

Consider the general quantum system having a time-dependent Hamiltonian of the form:

$$H(\underset{\sim}{r},t) = H^0(\underset{\sim}{r}) + 2FV(\underset{\sim}{r})\ T(t) \qquad \text{(VIII-49)}$$

where $H^0(\underset{\sim}{r})$ and $V(\underset{\sim}{r})$ are spatial operators, F is a parameter and $T(t)$ is a time-dependent function which we may leave unspecified for the time being.

Let $H^0(\underset{\sim}{r})$ have orthonormal eigenfunctions, $\psi_j(\underset{\sim}{r})$. W_j is the eigenvalue associated with the eigenfunction $\psi_j(\underset{\sim}{r})$:

$$H^0(\underset{\sim}{r})\psi_j(\underset{\sim}{r}) = W_j\psi_j(\underset{\sim}{r}) \qquad \text{(VIII-50)}$$

If we set $\hbar = 1$, the description of the system's quantum mechanical motion may be obtained by solving the Schrödinger differential equation:

$$i\dot{\Psi}(\underset{\sim}{r},t) = H(\underset{\sim}{r},t)\Psi(\underset{\sim}{r},t) \qquad \text{(VIII-51)}$$

after we have specified $\Psi(\underset{\sim}{r},t_0)$: the state of the system at the initial time t_0 .

We assume throughout that both H^0 and V are hermitian operators. This stipulation means that when applying the

Langhoff-Epstein-Karplus formalism to the Hamiltonian defined by Eq. (I-1), we must let $\gamma_a = \gamma_b = 0$.

We are concerned with solutions to the time-dependent Schrodinger Equation which obey the following initial condition:

$$\Psi(\underset{\sim}{r},t_0) = \psi_0(\underset{\sim}{r})e^{-iW_0t_0} \qquad \text{(VIII-52)}$$

where $\psi_0(r)$ is a <u>non-degenerate</u> eigenfunction of Eq. (VIII-50), W_0 is its non-degenerate eigenvalue and t_0 is the initial time of interest. The key idea in the Langhoff-Epstein-Karplus formalism is that the solutions which

(a) obey the initial conditions given by Eq. (VIII-52)

(b) result from an adiabatically turned-on periodic perturbation

may be written:

$$\Psi(\underset{\sim}{r},t) = \eta_0(t)\Phi(\underset{\sim}{r},t)e^{-iW_0t} \qquad \text{(VIII-53)}$$

The relationship between Eq. (VIII-53) and the usual Dirac variation of constants solution is easy to discuss. Let the Dirac expansion of the wavefunction be written as

$$\Psi(\underset{\sim}{r},t) = \sum_j \eta_j(t)\psi_j(\underset{\sim}{r})e^{-iW_0t} \qquad \text{(VIII-54)}$$

where j ranges over <u>all</u> eigenstates of $H^0(\underset{\sim}{r})$. Comparison of Eqs. (VIII-53) and (VIII-54) allows us to identify η_0 in (VIII-53) as the expansion coefficient of $\psi_0(\underset{\sim}{r})$ in (VIII-54). The time- and space-dependent function $\Phi(\underset{\sim}{r},t)$ is given by:

$$\Phi(\underset{\sim}{r},t) = \psi_0(\underset{\sim}{r}) + \sum_{j\neq 0} \frac{\eta_j(t)}{\eta_0(t)} \psi_j(\underset{\sim}{r}) \qquad \text{(VIII-55)}$$

Thus, the factorization of $\Psi(\underset{\sim}{r},t)$ given by Eq. (VIII-53) is equivalent to factoring out the expansion coefficient of $\psi_0(r)$ in the Dirac expansion. The purpose of the factorization is to include any over-all normalization and time-dependent phase factors in the function $\eta_0(t)$. We will have more to say of this later.

Substituting Eq. (VIII-53) into the time-dependent Schrödinger equation, we obtain a non-linear, first order differential equation for $\Phi(\underset{\sim}{r},t)$. Knowledge of $\Phi(\underset{\sim}{r},t)$ completely determines $\eta_0(t)$ and therefore solution of the equation for $\Phi(\underset{\sim}{r},t)$ is equivalent to the solution of the original Schrödinger Equation for $\Psi(\underset{\sim}{r},t)$. To demonstrate all of this, substitute expression (VIII-53) into Eq. (VIII-51) to obtain:

$$\dot{\Phi}(\underset{\sim}{r},t) + [\frac{\dot{\eta}_0(t)}{\eta_0(t)} - iW_0 + iH(\underset{\sim}{r},t)]\Phi(\underset{\sim}{r},t) = 0 \qquad \text{(VIII-56)}$$

From Eq. (VIII-55) we have

$$<\psi_0(\underset{\sim}{r})|\Phi(\underset{\sim}{r},t)> = 1 \; ; \quad <\psi_0(\underset{\sim}{r})|\dot{\Phi}(\underset{\sim}{r},t)> = 0 \qquad \text{(VIII-57)}$$

where the bra-ket notation is used to denote an integration over spatial coordinates:

$$\langle\psi_0(\underset{\sim}{r})|\phi(\underset{\sim}{r},t)\rangle = \int \psi_0^*(\underset{\sim}{r})\phi(\underset{\sim}{r},t)d\underset{\sim}{r}$$

Therefore, left multiplication of Eq. (VIII-56) by $\psi_0^*(\underset{\sim}{r})$ and subsequent spatial integration gives:

$$\frac{\dot{\eta}_0(t)}{\eta_0(t)} = -2iFI(t) \qquad \text{(VIII-58)}$$

where

$$I(t) \equiv T(t)\langle\psi_0(\underset{\sim}{r})|V(\underset{\sim}{r})\phi(\underset{\sim}{r},t)\rangle$$

Noting that the initial condition on $\eta_0(t)$ is

$$\eta_0(t_0) = 1$$

we write the appropriate particular solution to Eq. (VIII-58) as:

$$\eta_0(t) = \exp[-2iF\int_{t_0}^{t} I(t')dt'] \qquad \text{(VIII-59)}$$

Thus, $\eta_0(t)$ is <u>completely</u> determined by $\phi(\underset{\sim}{r},t)$ and we rewrite the expression for $\psi(\underset{\sim}{r},t)$ as:

$$\Psi(\underset{\sim}{r},t) = \Phi(\underset{\sim}{r},t)\exp[-iW_0 t - 2iF \int_{t_0}^{t} I(t')dt'] \quad \text{(VIII-60)}$$

To find the differential equation for $\Phi(\underset{\sim}{r},t)$, substitute Eq. (VIII-60) into Eq. (VIII-51) to obtain:

$$i\dot{\Phi}(\underset{\sim}{r},t) = [H(\underset{\sim}{r},t) - W_0]\Phi(\underset{\sim}{r},t) - 2FI(t)\Phi(\underset{\sim}{r},t) \quad \text{(VIII-61)}$$

Solution of Eq. (VIII-61) is equivalent to solution of the original Schrödinger Equation: Eq. (VIII-51). The non-linear structure of Eq. (VIII-61) is made more apparent by rewriting the expansion for $\Phi(\underset{\sim}{r},t)$ (Eq. (VIII-55)) as

$$\Phi(\underset{\sim}{r},t) = \psi_0(\underset{\sim}{r}) + \sum_{j\neq 0} b_j(t)\psi_j(\underset{\sim}{r}) \quad \text{(VIII-62)}$$

where

$$b_j(t) = \frac{\eta_j(t)}{\eta_0(t)} .$$

Substituting (VIII-62) into (VIII-61) we find the following set of first order non-linear equations for the b_k's $(k \neq 0)$:

$$\begin{aligned} i\dot{b}_k = {} & (W_k - W_0)b_k + 2FT(t)[V_{k0} - V_{00}b_k] \\ & + 2FT(t) \sum_{j\neq 0} b_j [V_{kj} - V_{0j}\, b_k] \end{aligned} \quad \text{(VIII-63)}$$

where

$$V_{ij} \equiv \langle\psi_i(r)|V(\underset{\sim}{r})\psi_j(\underset{\sim}{r})\rangle \ .$$

Purpose of Langhoff-Karplus-Epstein Formulation

The purpose of the formulation we have just described is two-fold. Firstly, it gives us a method of computing the part of $\Psi(\underset{\sim}{r},t)$ which alone is needed in computing properties: $\Phi(\underset{\sim}{r},t)$. To see this, assume that we wish to find the expectation value of the quantum mechanical operator $\bar{P}(r,t)$ where $\bar{P}(\underset{\sim}{r},t)$ contains no time derivatives.* The expectation value of $\bar{P}(\underset{\sim}{r},t)$ is given by

$$P(t) = \frac{\langle\Psi(\underset{\sim}{r},t)|\bar{P}(\underset{\sim}{r},t)|\Psi(\underset{\sim}{r},t)\rangle}{\langle\Psi(\underset{\sim}{r},t)|\Psi(\underset{\sim}{r},t)\rangle} \qquad \text{(VIII-64)}$$

If $\Psi(\underset{\sim}{r},t)$ is given by (VIII-53), we have:

$$P(t) = \frac{\int\Phi^*(\underset{\sim}{r},t)\bar{P}(\underset{\sim}{r},t)\Phi(\underset{\sim}{r},t)d\underset{\sim}{r}}{\int\Phi^*(\underset{\sim}{r},t)\Phi(\underset{\sim}{r},t)d\underset{\sim}{r}} \qquad \text{(VIII-65)}$$

and therefore only the function $\Phi(\underset{\sim}{r},t)$ is needed to compute such properties.

The second purpose of the formulation is concerned with the particular solutions of the Schrödinger Equation which corresponds

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* This restriction may be released by hermitizing the time-derivative operator. See footnote 33 in the Langhoff, Epstein, and Karplus review article.

to the steady-state response to an adiabatically turned-on periodic perturbation. When we use the present formulation to obtain the steady-state solutions as perturbation series in the parameter F, we expect the following convenient form:

(a) $\Phi(\underset{\sim}{r},t) = \Phi(\underset{\sim}{r},t+\frac{2\pi}{\omega})$ and $\Phi(\underset{\sim}{r},t)$ has no terms in it proportional to $(1/\omega)$

(b) $\eta_0(t) = \exp[\theta(t)]$ where <u>all</u> secular terms and all terms proportional to $(1/\omega)$ are included in $\theta(t)$.

A point we wish to emphasize is that, in general, only the steady-state solutions for a periodic perturbation will have the above convenient form. We demonstrate this by using the two-state system in a periodic perturbation as an example.

Consider the solution to (I-2) which obeys:*

$$\Psi(\underset{\sim}{r},0) = \psi_a(\underset{\sim}{r}) \qquad \text{(VIII-66)}$$

By Floquet's theorem the solution will be:

$$\begin{aligned}\Psi(\underset{\sim}{r},t) = &(C_1e^{-i\mu_1 t}\phi_{a1}(t) + C_2e^{-i\mu_2 t}\phi_{a2}(t))\psi_a(\underset{\sim}{r}) \\ &+ (C_1e^{-i\mu_1 t}\phi_{b1}(t) + C_2e^{-i\mu_2 t}\phi_{b2}(t))\psi_b(\underset{\sim}{r})\end{aligned} \qquad \text{(VIII-67)}$$

---

* Recall that we have stipulated $\gamma_a = \gamma_b = 0$.

where μ_1 and μ_2 are real constants, $\phi_{ij}(t + \frac{2\pi}{\omega}) = \phi_{ij}(t)$ and C_1 and C_2 are constants which will in general be non-vanishing if the initial condition in Eq. (VIII-66) is to be obeyed.

We can always factor Eq. (VIII-67) according to (VIII-53). The function $\Phi(\underset{\sim}{r},t)$ in this factorization will only be periodic, however, when either C_1 or C_2 is set equal to zero, i.e. when the initial conditions are such that the system starts off in a Floquet Mode.*

So then, in terms of the vocabulary used in this report, the underlying ideas in the Langhoff-Epstein-Karplus treatment are:

(a) Turning a periodic perturbation on adiabatically brings the system into initial conditions at $t = 0$ which give rise to a Floquet Normal Mode.

(b) The steady-state solutions are just the Floquet Normal Modes of a quantum system.

We now demonstrate these underlying ideas by using the two-state quantum system as an example.

<u>Example: Two-State Quantum System</u>

Consider the Hamiltonian defined by Eq. (VIII-49). Let $H^0(\underset{\sim}{r})$ have two orthonormal quantum states:

$$H^0(\underset{\sim}{r})\psi_j(\underset{\sim}{r}) = W_j\psi_j(\underset{\sim}{r}) \qquad j = a,b \ .$$

---

* This statement is true as long as μ_1 does not accidentally equal μ_2 .

The operator $V(r)$ has real matrix elements defined by

$$\langle\psi_k(\underset{\sim}{r})|V(\underset{\sim}{r})|\psi_\ell(\underset{\sim}{r})\rangle = V_{k\ell}$$

$T(t)$ is defined by

$$T(t) = e^{st} \cos\omega t \qquad \text{(VIII-68)}$$

where s is a real positive parameter. We consider $t_0 = -\infty$ and look for the state of the system at $t = 0$. We then let the parameter s go to zero. The multiplicative factor, $\exp(st)$, plays the role of a switching function which, in the limit of s going to zero, turns the harmonic perturbation on adiabatically.

To clarify the role of the switching function, consider the case of large s. Here, $T(t)$ is not large until t is very close to zero. The smaller the value of s, however, the more slowly the perturbation is turned on. In the limit of s going to zero, the $\cos\omega t$ perturbation will be turned on adiabatically* (with infinite slowness).

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* There is a problem with this form of the switching function. Namely:

$$\lim_{s \to 0} \left[\frac{d}{dt} T(t)\right] \neq 0 \, .$$

We overlook this difficulty, however, since it does give us the desired particular solution for $\Phi(\underset{\sim}{r},t)$ $(t > 0)$ which contains only the frequencies ω and $n\omega$ (n integer).

Using Eq. (VIII-68) in Eq. (VIII-61), we solve the resulting equation by a perturbation expansion in the field strength:

$$\Phi(\underset{\sim}{r},t) = \sum_{n=0}^{\infty} F^n \, \Phi^{(n)}(\underset{\sim}{r},t)$$

and require $\Phi(\underset{\sim}{r},t_0) = \psi_a(\underset{\sim}{r})$ where $t_0 = -\infty$. In terms of the series expansion of $\Phi(\underset{\sim}{r},t)$, we require:

$$\Phi^{(n)}(\underset{\sim}{r},t_0) = \psi_a \delta_{n0} \; ; \quad t_0 = -\infty \, . \qquad \text{(VIII-69)}$$

For example, the zeroth order equation

$$i\dot{\Phi}^{(0)}(\underset{\sim}{r},t) = H^{(0)}(\underset{\sim}{r})\Phi^{(0)}(\underset{\sim}{r},t) - W_a\Phi^{(0)}(\underset{\sim}{r},t) \qquad \text{(VIII-70)}$$

is already satisfied by our choice:

$$\Phi^{(0)}(\underset{\sim}{r},t) = \psi_a(\underset{\sim}{r}) \, . \qquad \text{(VIII-71)}$$

The equation for $\Phi^{(1)}(\underset{\sim}{r},t)$ is:

$$i\dot{\Phi}^{(1)}(\underset{\sim}{r},t) = (H^{(0)}(\underset{\sim}{r}) - W_a)\Phi^{(1)}(\underset{\sim}{r},t) + 2V(\underset{\sim}{r})e^{st}\cos\omega t\psi_a(\underset{\sim}{r}) - 2V_{aa}e^{st}\cos\omega t\psi_a(\underset{\sim}{r}) \qquad \text{(VIII-72)}$$

By assuming the Dirac expansion:

$$\Phi^{(1)}(\underset{\sim}{r},t) = \Lambda_a^{(1)}(t)\psi_a(\underset{\sim}{r}) + \Lambda_b^{(1)}(t)\psi_b(\underset{\sim}{r})$$

we find the following equations for the time-dependent coefficients:

$$\dot{\Lambda}_a^{(1)} = 0 \ ; \quad i\dot{\Lambda}_b^{(1)} = \Delta W\Lambda_b^{(1)} + 2V_{ab}\, e^{st}\cos\omega t \qquad \text{(VIII-73)}$$

where $\Delta W \equiv W_b - W_a$. We easily solve these equations and we determine the constants of integration by using Eq. (VIII-69). Doing so, we obtain:

$$\Phi^{(1)} = -V_{ab}\, e^{st}\left[\frac{e^{i\omega t}}{\Delta W+\omega-is} + \frac{e^{-i\omega t}}{\Delta W-\omega-is}\right]\psi_b(\underset{\sim}{r}) \qquad \text{(VIII-74)}$$

We continue in an exactly similar fashion to find:

$$\Phi^{(2)} = \Delta V V_{ab}\, e^{2st}\left[\begin{aligned}&\frac{1}{(\Delta W+\omega-is)}\left[\frac{e^{2i\omega t}}{\Delta W+2\omega-2is} + \frac{1}{\Delta W-2is}\right]\\ &+ \frac{1}{(\Delta W-\omega-is)}\left[\frac{e^{-2i\omega t}}{\Delta W-2\omega-2is} + \frac{1}{\Delta W-2is}\right]\end{aligned}\right]\psi_b(\underset{\sim}{r})$$

(VIII-75)

where $\Delta V = V_{bb} - V_{aa}$. We find even higher order correction in an exactly similar fashion.

Since $\Psi(\underset{\sim}{r},t)$ is completely specified by use of Eq. (VIII-60), we need now to merely evaluate the integral:

$$-2iF\int_{-\infty}^{t} dt'\; e^{st'}\cos\omega t' \langle \psi_a(\underset{\sim}{r}) | V(\underset{\sim}{r}) | \Phi^{(0)}(\underset{\sim}{r},t) + F\Phi^{(1)}(\underset{\sim}{r},t) + \ldots \rangle$$

$$= FE^{(1)} + F^2E^{(2)} + \ldots$$

We find that

$$E^{(1)} = -iV_{aa}\; e^{st}\left[\frac{e^{i\omega t}}{s+i\omega} + \frac{e^{-i\omega t}}{s-i\omega}\right]$$

$$E^{(2)} = \frac{i(V_{ab})^2\; e^{2st}}{2}\left[\frac{1}{\Delta W+\omega-is}\left[\frac{e^{2i\omega t}}{s+i\omega} + \frac{1}{s}\right] + \frac{1}{\Delta W-\omega-is}\left[\frac{e^{-2i\omega t}}{s-i\omega} + \frac{1}{s}\right]\right]$$

(VIII-76)

Accumulating results we have

$$\Psi(\underset{\sim}{r},t) = [\psi_a + F\Phi^{(1)} + F^2\Phi^{(2)} + \ldots]\exp[-iW_a t + FE^{(1)} + F^2E^{(2)} + \ldots]$$

(VIII-77)

where $\Phi^{(1)}$ and $\Phi^{(2)}$ are respectively given by Eqs. (VIII-74) and (VIII-75). $E^{(1)}$ and $E^{(2)}$ are given by (VIII-76). We are now interested in using Eq. (VIII-77) to find

$$\lim_{s\to 0} \Psi(\underset{\sim}{r},0)$$

This will give us the initial conditions appropriate to the "steady-state" solution. Taking the limit of each and every term is trivial except for the term $E^{(2)}(0)$:

$$\mathcal{E}^{(2)}(0) = \frac{i(V_{ab})^2}{2}\left[\frac{1}{\Delta W+\omega-is}\left[\frac{1}{s+i\omega} + \frac{1}{s}\right] + \frac{1}{\Delta W-\omega-is}\left[\frac{1}{s-i\omega} + \frac{1}{s}\right]\right] \quad \text{(VIII-78)}$$

The bothersome terms in $\mathcal{E}^{(2)}(0)$ are terms proportional to $(1/s)$. They are handled, however, by looking at the following refactorization of $\mathcal{E}^{(2)}(0)$:

$$\lim_{s \to 0} [\mathcal{E}^{(2)}(0)] = \frac{-2(V_{ab})^2[(\Delta W)^2 + \omega^2]}{[(\Delta W)^2 - \omega^2]^2}$$

(VIII-79)

$$+ \frac{i(V_{ab})^2}{2} \lim_{s \to 0} \left[\frac{\Delta W+\omega}{s[(\Delta W+\omega)^2 + s^2]} + \frac{\Delta W-\omega}{s[(\Delta W-\omega)^2 + s^2]}\right]$$

In the refactorization, there is still a term going as $(s)^{-1}$. Note, however, that although this term is indeterminate as s goes to zero, it is an indeterminate <u>pure imaginary</u> number. This term appears as multiplying $\Psi(\underset{\sim}{r},0)$ by $\exp(i\xi)$ where ξ is some indeterminate real number. This term can be thought of as an undetermined time-independent phase factor and it can therefore be ignored. We will then take

$$\lim_{s \to 0} \mathcal{E}^{(2)} = -\frac{2(V_{ab})^2[(\Delta W)^2 + \omega^2]}{[(\Delta W)^2 - \omega^2]^2}$$

and thereby ignore this phase factor in computing the final result.

With the limits taken, we find the following initial condition appropriate to the steady-state wavefunction:

$$\Psi(\underset{\sim}{r},0) = e^{\bar{\theta}_1'} \psi_a + \bar{\Phi}_1' \psi_b e^{\bar{\theta}_1'}$$

where

$$\bar{\theta}_1' = -\frac{2F^2(V_{ab})^2[\Delta W^2 + \omega^2]}{[\Delta W^2 - \omega^2]} + F^3 \ldots$$

(VIII-80)

$$\bar{\Phi}_1' = -\frac{2FV_{ab}\Delta W}{(\Delta W)^2 - \omega^2} + F^2\Delta VV_{ab}\left[\frac{2}{\Delta W^2-\omega^2} + \frac{1}{(\Delta W+\omega)(\Delta W+2\omega)} + \frac{1}{(\Delta W-\omega)(\Delta W-2\omega)}\right]$$
$$+ F^3 \ldots$$

But note that aside from a normalization factor, Eq. (VIII-80) give the same initial conditions which are obeyed by the Floquet Normal Mode solution given by Eq. (VIII-46).

We, therefore, conclude that if the two-level system is in quantum state $\psi_a(\underset{\sim}{r})$ before the harmonic perturbation is adiabatically turned-on, at $t = 0$ the system will be in the Floquet Normal Mode solution which corresponds to

$$\lim_{F \to 0} \eta_a(0) = 1 \; ; \qquad \lim_{F \to 0} \eta_b(0) = 0$$

where η_a and η_b are defined by Eq. (I-3).

Carrying out an exactly similar analysis, we find that if the two-level system is in quantum state $\psi_b(\underset{\sim}{r})$ at $t = -\infty$, an adiabatic turn-on of the harmonic perturbation yields the other

Floquet Normal Mode solution at $t > 0$: namely, the Floquet solution corresponding to:

$$\lim_{F \to 0} \eta_a(0) = 0 \; ; \qquad \lim_{F \to 0} \eta_b(0) = 1$$

We have therefore given a simple example which demonstrate the assertion that the steady-state solutions of a general quantum system may be defined in the following simple manner:

If a quantum system is in the non-degenerate quantum state $\psi_j(r)$, an adiabatic turn-on of a $\cos\omega t$ perturbation puts the system in the Floquet state:

$$\Psi_F(\underset{\sim}{r},t) = \hat{\Phi}(\underset{\sim}{r},t)e^{-i\mu t}$$

where μ is a constant, $\hat{\Phi}(\underset{\sim}{r},t + \frac{2\pi}{\omega}) = \hat{\Phi}(\underset{\sim}{r},t)$ and, if E_j is the eigenvalue associated with $\psi_j(\underset{\sim}{r})$,

$$\lim_{F \to 0} \Psi_F(\underset{\sim}{r},t) = \psi_j(\underset{\sim}{r})e^{-iE_j t}$$

The Convergence of the Steady-State Solutions

Expressed as a Power Series in F

We have already discussed the conditions we must impose if (VIII-46) and (VIII-47) are to converge. These conditions are detailed by (VIII-48) and they are, therefore, conditions which we must impose on the steady-state results if they are to quickly converge. There is a problem, however. The steady-state solutions are successfully used in the theoretical computation of optical properties in the entire region of $0 \leq \omega < \Delta W$ and because of criteria (VIII-48) we would not expect this to be so. For instance we would expect the steady-state solutions to be poor approximations when

Case (a). ω is very, very small.

(Case(b). $\Delta W/\omega$ approximately (or exactly) equals some positive integer n .

Case (a).

When ω is very, very small, no matter how small the field strength, F , is, we would expect FV_{ij}/ω $(i,j = a,b)$ to be of order unity or larger in some region of very small ω . In this instance, the steady-state solutions do not quickly converge.

Case (b).

If $\Delta W/\omega \simeq n$, a denominator in the n-th order of perturbation would almost equal zero. This would clearly not give rise to a quickly converging approximation.

How can we reconcile the fact that the steady-state perturbation technique gives results in agreement with experiment when we claim that it should not in Cases (a) and (b)?

In Case (a), we can resolve the apparent contradiction by remembering that we are talking about using (VIII-27) and (VIII-28) to compute average values of properties, P . Therefore, we are looking at expressions of the form

$$P(t) = \frac{\int \Psi^*(\underset{\sim}{r},t)\bar{P}(\underset{\sim}{r})\Psi(\underset{\sim}{r},t)d\underset{\sim}{r}}{\int \Psi^*(\underset{\sim}{r},t)\Psi(\underset{\sim}{r},t)d\underset{\sim}{r}} \qquad \text{(VIII-81)}$$

Where $P(t)$ is the time-dependent expectation value of the spatial quantum mechanical operator $\bar{P}(\underset{\sim}{r})$. Consider the particular solution given by (VIII-46). For this case

$$\Psi(\underset{\sim}{r},t) = \psi_a(\underset{\sim}{r})e^{\theta_1'} + \psi_b(\underset{\sim}{r})\Phi_1' e^{\theta_1'} \qquad \text{(VIII-82)}$$

Using (VIII-82) in (VIII-81) we obtain

$$\bar{P}(t) = \frac{[\bar{P}_{aa} + 2\text{Re}[\bar{P}_{ab}\Phi_1'] + \bar{P}_{bb}(\Phi_1')^*(\Phi_1')]}{1 + (\Phi_1')^*(\Phi_1')} \qquad \text{(VIII-83)}$$

where

$$\bar{P}_{ij} \equiv \int \psi_i^*(\underset{\sim}{r})\bar{P}(\underset{\sim}{r})\psi_j(\underset{\sim}{r})d\underset{\sim}{r}$$

Since $P(t)$ is an observable, it is pure real and furthermore, it does not involve θ_1' . Since <u>only</u> θ_1' contains terms in inverse powers of ω , $P(t)$ contains <u>no</u> terms in $(\omega)^{-1}$. Therefore, the restriction imposed by Case (a) can be ignored when average values of <u>properties</u> are computed. We obtain the interesting result that we may obtain a quickly converging result for a property with a wavefunction which is slowly convergent or divergent.

If we consider the particular solution given by (VIII-28),

$$\Psi(\underset{\sim}{r},t) = \psi_a(\underset{\sim}{r})\Phi_2' e^{\theta_2'} + \psi_b(\underset{\sim}{r}) e^{\theta_2'}$$

and substitute it into (VIII-30), we also find that since terms in $(\omega)^{-1}$ appear only in $\theta_2'(t)$, these terms do not appear in $P(t)$.

These observations are not new. They are discussed in the Langhoff-Epstein-Karplus review article.

Now, what about the difficulty described by Case (b)? We would expect that denominators of the form

$$\Delta W - n\omega$$

would make $P(t)$ non-converging when such denominators are zero or almost zero. This difficulty has been pointed out to Epstein and he has suggested* that even though we do not expect convergence of the series for $\omega < \Delta W$ because of the appearance of denominators which are approximately zero the low order results may have some sort of relevance since if $\omega << \Delta W$ the "bad" denominators will not appear until very high order in the perturbation theory. We therefore conclude that the series is asymptotically convergent.

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* S. T. Epstein, private communication.

IX. TECHNIQUE T5: DEGENERATE RAYLEIGH-SCHRÖDINGER PERTURBATIONS: $\alpha \approx \beta \approx \varepsilon \approx \delta$ AND ALL ARE MUCH LESS THAN UNITY

In (VII-13) we gave the convergence conditions for the solution of (V-5) by a non-degenerate Rayleigh-Schrödinger expansion in the field strength. The case of α, β, ε and δ all having the same magnitude and all being much less than one:

$$\alpha \approx \beta \approx \varepsilon \approx \delta << 1 \qquad \text{(IX-1)}$$

was not covered by (VII-13). This is because the conditions given in (IX-1) would give rise to expansion coefficients, the $C_{k,j}^{(n)}$'s of (VII-7), which would involve factors of the form

$$\frac{\alpha}{\varepsilon - i\delta}, \quad \frac{\beta}{\varepsilon - i\delta}$$

These factors are clearly of order unity if the conditions (IX-1) hold. If the expansion coefficients are of order unity, we would not expect the perturbation series to quickly converge.

We can easily overcome this difficulty by splitting up H_F in a new way. The problem with splitting up H_F into a part independent to the field strength and a part directly proportional to the field strength (i.e. the split-up given by (VII-2) and (VII-3)) is that when both ε and δ are very, very small, some of the zeroth order eigenvalues are almost degenerate. For instance the zeroth order energy associated with $|B,j\rangle$ differs from the zeroth order energy associated with $|A,j\rangle$ by the quantity $\pm(\varepsilon - i\delta)$ which, by hypothesis, is very, very small. In the new split-up of H_F, we will make the zeroth order energies exactly rather than almost degenerate. This process is the text-book method of treating the difficulty of an almost-degenerate zeroth-order Hamiltonian. For example, Messiah (1964) discusses this general technique in Vol. 2, p. 711. Certain (1970b), Dion and Hirschfelder give a simple example of this procedure.

As far as we know, no other authors have applied this technique to the specific problem of the two-level quantum system in a $\cos\omega t$ field. This is not surprising, since the conditions given by (IX-1) seldom arise. For example, if $\varepsilon \ll 1$, ω must be such that it is much greater than all of the resonance frequencies of the system. This is clearly a regime of ω which is not of great physical interest.

The first step in Technique T5 is to split H_F (defined by (V-2)) in the following manner:

$$H_F = \bar{H}_F^{(0)} + \lambda \bar{H}_F^{(1)} \qquad \text{(IX-2)}$$

where λ is again an ordering parameter which will be set equal to unity at the end of the calculation. Bars have been put on $\bar{H}_F^{(0)}$ and $\bar{H}_F^{(1)}$ to distinguish them from the "unbarred" operators, $H_F^{(0)}$ and $H_F^{(1)}$, which were defined by (VII-2) and (VII-3) respectively.

$\bar{H}_F^{(0)}$ is defined by

$$\bar{H}_F^{(0)}|k,j> \;=\; j|k,j> \qquad k = A \text{ or } B \tag{IX-3}$$

$\bar{H}_F^{(0)}$ is a hermitian operator, whereas, $\bar{H}_F^{(1)}$ is a non-hermitian operator:

$$\begin{aligned} \bar{H}_F^{(1)}|A,j> &= \alpha[|B,j+1> + |B,j-1>] \\ \bar{H}_F^{(1)}|B,j> &= \alpha[|A,j+1> + |A,j-1>] + (\varepsilon - i\delta)|B,j> \\ &\quad + \beta[|B,j+1> + |B,j-1>] \end{aligned} \tag{IX-4}$$

Note that $\bar{H}_F^{(0)}$ has degenerate eigenvalues since, $|A,j>$ and $|B,j>$ have the same eigenvalue with respect to $\bar{H}_F^{(0)}$.

We again wish to solve the Schrödinger-type equation .

$$H_F|\mu> \;=\; \mu|\mu> \tag{IX-5}$$

by assuming that both the eigenvalue, μ , and the eigenvector, $|\mu>$, can be expanded in a power series in λ :

$$\mu = \sum_{n=0}^{\infty} \lambda^n \mu^{(n)} \;; \qquad |\mu> = \sum_{n=0}^{\infty} \lambda^n |\mu^{(n)}> \tag{IX-6}$$

We can substitute the expansion (IX-6) and the split-up of H_F given by (IX-2) into (IX-5). After regrouping terms in similar powers of λ, we can obtain a solvable set of perturbation equations. These must be solved by degenerate Rayleigh-Schrödinger perturbation theory.*

Once we obtain solutions to the static problem (IX-5), we can recover the solutions to the dynamic problem of (II-4) and (II-5) by utilizing the equivalence of the two problems described by (V-7) and (V-8).

The zeroth order degenerate Rayleigh-Schrödinger equation is:

$$\bar{H}_F^{(0)}|\mu^{(0)}\rangle = \mu^{(0)}|\mu^{(0)}\rangle \qquad \text{(IX-7)}$$

It has as its most general solution

$$|\mu^{(0)}\rangle = C_A^{(0)}|A,j\rangle + C_B^{(0)}|B,j\rangle$$

and

$$\mu^{(0)} = j$$

where $C_A^{(0)}$ and $C_B^{(0)}$ are constants which will be determined by the first order perturbation equation. Since the final time-dependent results are invariant to the choice of j, let us, for the sake of simplicity, take $j = 0$. We therefore have

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* For a discussion of degenerate Rayleigh-Schrödinger perturbation theory see Schiff (1955), Pauling and Wilson (1935) or any other elementary Quantum Mechanics text.

$$|\mu^{(0)}> = C_A^{(0)}|A,0> + C_B^{(0)}|B,0>$$
$$\mu^{(0)} = 0 \qquad \text{(IX-8)}$$

The constants, $C_A^{(0)}$ and $C_B^{(0)}$, as well as the first order energy, $\mu^{(1)}$, are determined from the first order perturbation equation:

$$\bar{H}_F^{(1)}|\mu^{(0)}> + \bar{H}_F^{(0)}|\mu^{(1)}> = \mu^{(1)}|\mu^{(0)}> + \mu^{(0)}|\mu^{(1)}> \qquad \text{(IX-9)}$$

Using (IX-8) in (IX-9) we obtain

$$\bar{H}_F^{(1)}(C_A^{(0)}|A,0> + C_B^{(0)}|B,0>) = \mu^{(1)}(C_A^{(0)}|A,0> + C_B^{(0)}|B,0>) \qquad \text{(IX-10)}$$
$$+ \bar{H}_F^{(0)}|\mu^{(1)}>$$

Equation (IX-10) may first be multiplied by $<A,0|$ and may then be multiplied by $<B,0|$ to obtain the following linear homogeneous system of equations:*

$$\mu^{(1)}C_A^{(0)} = 0$$
$$\mu^{(1)}C_B^{(0)} = C_B^{(0)}(\varepsilon - i\delta) \qquad \text{(IX-11)}$$

The system (IX-11) has a two non-trivial, normalized solutions:

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* To obtain Eq. (IX-11), we use that fact that since $|\mu^{(1)}>$ may by expanded in the ortho-normal $\{|A,j>,|B,j>\}$ basis we have:

$$<k,0|\bar{H}_F^{(0)}|\mu^{(1)}> = 0 \qquad (k = A \text{ or } B) .$$

$$\underline{\text{Choice I}}: \quad \mu^{(1)} = 0 \,, \quad C_A^{(0)} = 1 \,, \quad C_B^{(0)} = 0$$

$$\underline{\text{Choice II}}: \quad \mu^{(1)} = (\varepsilon - i\delta) \,, \quad C_A^{(0)} = 0 \,, \quad C_B^{(0)} = 1 \qquad \text{(IX-12)}$$

The degeneracy has therefore been broken in the first order of the perturbation and the higher order corrections may easily be obtained. We will find that the solution to (IX-5) arising from Choice I will give rise to one of the Floquet Normal Modes. The solution arising from Choice II will give rise to the other Floquet Normal Mode.

For example, let us consider Choice I. Put the subscript "1" on the perturbation eigenvalues, $\mu^{(n)}$, and the perturbation eigenvectors, $|\mu^{(n)}>$, to indicate that they arise from Choice I. Therefore,

$$|\mu_1^{(0)}> \;=\; |A,0> \,, \quad \mu_1^{(0)} = 0 \,, \quad \mu_1^{(1)} = 0 \,.$$

The first order equation, equation (IX-9), becomes

$$\bar{H}_F^{(1)}|A,0> + \bar{H}_F^{(0)}|\mu_1^{(1)}> \;=\; 0 \qquad \text{(IX-13)}$$

In solving (IX-13), we must resolve the question of normalization. We can choose the component of $|\mu_1^{(0)}>$ in $|\mu_1^{(n)}>$ (where $n \geq 1$) to be anything we want. We will make the following simple choice:

$$<\mu_1^{(0)}|\mu_1^{(n)}> \;=\; \delta_{n,0} \qquad \text{(IX-14)}$$

If $|\mu_2^{(0)}>$ is the Choice II zeroth order wavefunction, $<\mu_2^{(0)}|\mu_1^{(1)}>$, is not determined by (IX-13). It is, however, determined by the equation for $|\mu_1^{(2)}>$.

To detail the T5 procedure, let $|\mu_1^{(1)}>$ be expanded in the spectrum of $\bar{H}_F^{(0)}$:

$$|\mu_1^{(1)}> \;=\; \sum_{k=A,B} \sum_{\ell=-\infty}^{\infty} c_{k,\ell}^{(1)}|k,\ell> \qquad \text{(IX-15)}$$

where the $c_{k,\ell}^{(1)}$'s are expansion coefficients. Substitution of Eq. (IX-15) into (IX-13) and subsequent left-multiplication of the result by each and every $<k,\ell|$, gives the following results:

(1) $c_{A,0}^{(1)}$ is zero by imposing Eq. (IX-14).

(2) $c_{B,0}^{(1)}$ is not determined by the first order equation.

(3) All other expansion coefficients vanish except $c_{B,1}^{(1)}$ and $c_{B,-1}^{(1)}$. The former is $-\alpha$ and the later is α .

We therefore have

$$|\mu_1^{(1)}> \;=\; c_{B,0}^{(1)}|B,0> + \alpha[|B,-1> - |B,1>] \qquad \text{(IX-16)}$$

where $c_{B,0}^{(1)}$ will be determined by the second order equation:

$$\bar{H}_F^{(0)}|\mu_1^{(2)}> + \bar{H}_F^{(1)}|\mu_1^{(1)}> \;=\; \mu_1^{(2)}|A,0> \qquad \text{(IX-17)}$$

We again assume that $|\mu_1^{(2)}>$ may be expanded in the $|A,j>;|B,j>$ basis

$$|\mu_1^{(2)}\rangle = \sum_{k=A,B}{}' \sum_{\ell=-\infty}^{\infty} c_{k,\ell}^{(2)} |k,\ell\rangle \qquad \text{(IX-18)}$$

where the $c_{k,\ell}^{(2)}$'s are expansion coefficients and the prime on the summation means that because of (IX-14) we will exclude the state $|A,0\rangle$ from the summation. Using (IX-18) in (IX-17), we left-multiply the result by $\langle A,0|$ to find

$$\mu_1^{(2)} = 0 .$$

Left-multiplication of the result by $\langle B,0|$ determines that $c_{B,0}^{(1)}$ vanishes. $c_{B,0}^{(2)}$, however, is not yet determined. Continuing this procedure with the other $\langle k,\ell|$'s , we find only six non-vanishing coefficients. The second order correction, therefore, is:

$$|\mu_1^{(2)}\rangle = c_{B,0}^{(2)}|B,0\rangle + \alpha(\varepsilon - i\delta)[|B,1\rangle + |B,-1\rangle] + \frac{\alpha^2}{2}[|A,2\rangle + |A,-2\rangle] + \frac{\alpha\beta}{2}[|B,2\rangle + |B,-2\rangle]$$

After making a spectral expansion of $|\mu_1^{(3)}\rangle$ and then substituting it into the third order equation, we determine $c_{B,0}^{(2)}$ and $\mu_1^{(3)}$ by left-multiplying the result by $\langle A,0|$ and $\langle B,0|$. Neither quantity vanishes and we find that

$$\mu_1^{(3)} = 2\alpha^2(\varepsilon - i\delta) \qquad c_{B,0}^{(2)} = -2\alpha\beta$$

This procedure may be continued to obtain a solution of arbitrary accuracy. We assemble the Choice I results (which are correct through third order in the energy and second order in the wavefunction) in the following expression:

$$\mu_1 = \lambda^3 2\alpha^2(\varepsilon - i\delta) + \ldots$$

$$|\mu_1> = |A,0> + \lambda\alpha[|B,-1> - |B,1>]$$

$$+ \lambda^2\left[\begin{array}{l}-2\alpha\beta|B,0> + \alpha(\varepsilon - i\delta)[|B,1> + |B,-1>] \\ + \frac{\alpha^2}{2}[|A,2> + |A,-2>] + \frac{\alpha\beta}{2}[|B,2> + |B,-2>]\end{array}\right] + \ldots. \qquad \text{(IX-19)}$$

Setting the ordering parameter, λ, equal to unity and utilizing (V-7) and (V-8) to obtain a time-dependent solution, we obtain one of the Floquet Normal Modes:

$$a_1 = e^{-i\mu_1\tau}\,\phi_{a1}(\tau)\ ; \quad b_1\ e^{-i\mu_1\tau}\,\phi_{b1}(\tau)$$

$$\mu_1 = 2\alpha^2(\varepsilon - i\delta) + \ldots \qquad \text{(IX-20)}$$

$$\phi_{a_1} = 1 + \alpha^2\cos(2\tau) + \ldots$$

$$\phi_{b1} = -2i\alpha\sin\tau - 2\alpha\beta + 2\alpha(\varepsilon - i\delta)\cos\tau + \alpha\beta\cos(2\tau) + \ldots$$

The second choice of $|\mu^{(0)}>$ and $\mu^{(1)}$ leads to the other Floquet Normal Mode:

$$a_2 = e^{-i\mu_2\tau}\phi_{a2}(\tau) \; ; \quad b_2 = e^{-i\mu_2\tau}\phi_{b2}(\tau)$$

$$\mu_2 = (\varepsilon - i\delta) - 2\alpha^2(\varepsilon - i\delta) + \ldots$$

$$\phi_{a2}(\tau) = -2i\alpha\sin\tau - 2\alpha(\varepsilon - i\delta)\cos\tau + \alpha\beta\cos(2\tau) + \ldots \qquad \text{(IX-21)}$$

$$\phi_{b2}(\tau) = 1 - 2i\beta\sin\tau + (\alpha^2 + \beta^2)\cos(2\tau) + \ldots$$

Inspection of (IX-20) and (IX-21), confirms the hypothesis that they should be quickly converging solutions for the Floquet Normal Modes when α, β, ε and δ are all much less than unity.

X. PARTITIONING TECHNIQUES FOR FIELD STRENGTH EXPANSIONS

Introduction

In order to obtain solutions for those cases where the zeroth order energy of the Floquet Hamiltonian is almost (or exactly) degenerate, we can use the standard partitioning perturbation techniques. Löwdin's (1966) procedures may be the most familiar but we shall describe how the Certain-Dion-Hirschfelder (1970a, 1970b, 1970c) version applies to the Floquet problem. In this way, when we solve

$$H_F|\mu> \; = \; \mu|\mu>$$

we obtain the wavefunction, $|\mu>$, accurate through the n-th order in the field strength and, correspondingly, the energy accurate through the (2n+1)-th order. However, this procedure is <u>not</u> a Rayleigh-Schrödinger perturbation since the energy is <u>not</u> expanded in a power series in the field strength.

General Considerations

In section VII we discussed the solution to (II-4) and (II-5) by splitting up the static Floquet Hamiltonian into a zeroth order part, $H_F^{(0)}$, which did not depend on the field strength and into a perturbation, $H_F^{(1)}$, which directly depended on the field strength. We saw that if we applied non-degenerate Rayleigh-Schrödinger perturbation theory to H_F

split up in this manner, the resulting solutions would only converge for certain ranges of the parameters α, β, ε and δ. Those ranges were given by (VII-13). The problem was that G (defined by (VII-8)) would be large for ranges of ε and δ which made the denominator in G very small. Suppose, for simplicity, that <u>only one</u> $(\mu^{(0)}_{k,n} - \mu^{(0)}_{k_0,n_0})$ in all of the possible G's is small enough to make the fraction G much larger than unity. Call it

$$(\mu^{(0)}_{k_1,n_1} - \mu^{(0)}_{k_0,n_0}) \qquad \text{(X-1)}$$

If we could somehow exclude the term involving the very small or vanishing quantity

$$(\mu^{(0)}_{k_1,n_1} - \mu^{(0)}_{k_0,n_0})$$

from all higher order corrections to the zeroth order eigenfunctions and eigenvalues, we would then obtain a quickly converging perturbation expansion. The technique which accomplishes this is partitioning perturbation theory. The technique is not restricted to the case of there being <u>only one</u> "bad denominator" of the form (X-1). For our purposes, however, we need only consider this case.

The bad denominator appeared in the non-degenerate Rayleigh-Schrödinger perturbation expansion because two zeroth order states, the states $|\mu^{(0)}_{k_1,n_1}>$ and $|\mu^{(0)}_{k_0,n_0}>$, had zeroth order energies which were almost (or exactly) degenerate.* This caused poorly converging higher order corrections. The idea behind partitioning is that instead of solving for <u>either</u> the perturbed state arising from $|\mu^{(0)}_{k_1,n_1}>$ <u>or</u> the perturbed state arising from $|\mu^{(0)}_{k_0,n_0}>$, we solve for the perturbed two component row vector, $\underset{\sim}{\chi}$, which arises from the zeroth order 1×2 now vector

$$\underset{\sim}{\chi}^{(0)} = (|\mu^{(0)}_{k_1,n_1}> , \ |\mu^{(0)}_{k_0,n_0}>) . \qquad \text{(X-2)}$$

As we will show, doing this we can avoid "bad denominators" of the form (X-1) appearing in the final energies and wavefunctions. Now what is this row vector $\underset{\sim}{\chi}$? To answer this question, let us first assume that we have solved

$$H_F|\mu_j> = \mu_j|\mu_j> \qquad j = 1,2 \qquad \text{(X-3)}$$

where μ_j is an eigenvalue of H_F and $|\mu_j>$ is its associated eigenvector. We can write these two Schrödinger equations in matrix notation:

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* For example, if $\delta = 0$ and $\varepsilon = 1$, the states $|\mu^{(0)}_{A,1}>$ and $|\mu^{(0)}_{B,0}>$ have <u>exactly</u> the same zeroth order energy.

$$H_F \underset{\sim}{\Psi} = \underset{\sim}{\Psi} \underset{\approx}{W} \tag{X-4}$$

where $\underset{\sim}{\Psi}$ is the two component row vector

$$\underset{\sim}{\Psi} = (|\mu_1\rangle , |\mu_2\rangle) . \tag{X-5}$$

In order that (X-3) be satisfied, we define $\underset{\approx}{W}$ to be the following 2×2 matrix:

$$\underset{\approx}{W} = \begin{pmatrix} \mu_1 & 0 \\ 0 & \mu_2 \end{pmatrix} \tag{X-6}$$

$\underset{\sim}{\chi}$ may now be defined in terms of $\underset{\sim}{\Psi}$: <u>the row vector $\underset{\sim}{\chi}$ is a two component vector, each component of which is a linear combination of two exact solutions to the Schrödinger Equation,</u> $|\mu_1\rangle$ <u>and</u> $|\mu_2\rangle$. In matrix notation, we may therefore write $\underset{\sim}{\chi}$ in terms of $\underset{\sim}{\Psi}$ and a 2×2 non-singular matrix of constants $\underset{\approx}{c}$:

$$\underset{\sim}{\chi} = \underset{\sim}{\Psi} \underset{\approx}{c} . \tag{X-7}$$

Since

$$\underset{\sim}{\Psi} = \underset{\sim}{\chi} \underset{\approx}{c}^{-1} , \tag{X-8}$$

we may use this expression for $\underset{\approx}{\Psi}$ in (X-4). We may then right multiply result by $\underset{\approx}{c}$ to obtain the following "scrambled" Schrodinger Equation:

$$H_F \underset{\sim}{\chi} = \underset{\sim}{\chi} \underset{\approx}{E} \tag{X-9}$$

where $\underset{\approx}{E}$ is a 2×2 matrix defined by:

$$\underset{\approx}{E} = \underset{\approx}{c}^{-1} \underset{\approx}{W} \underset{\approx}{c} \tag{X-10}$$

In partitioning perturbation theory, we solve equation (X-9) (which is a "scrambled" Schrödinger equation) rather than the Schrödinger equation itself (equation (X-4)). We will find that if we perturbatively solve (X-9) we may avoid the "bad denominators" which appear in the straightforward non-degenerate Rayleigh-Schrödinger perturbation solution of (X-4).

Exact Solution of (X-9)

Assume we have solved (X-9). We therefore know $\underset{\sim}{\chi}$:

$$\underset{\sim}{\chi} = (|\chi_a> , |\chi_b>) \tag{X-11}$$

where we have written out the (1,1) component of $\underset{\sim}{\chi}$ as $|\chi_a>$ and its (1,2) component as $|\chi_b>$. $\underset{\approx}{E}$ will be a 2×2 matrix and it is not necessarily hermitian. The 2×2 matrix $\underset{\approx}{c}$ which relates $\underset{\sim}{\chi}$ to $\underset{\sim}{\Psi}$ is not necessarily unitary. If $\delta = 0$, however, H_F becomes a Hermitian operator. In this case, we make $\underset{\approx}{E}$ hermitian and $\underset{\approx}{c}$ unitary by specifying that $\underset{\sim}{\chi}$ is normalized according to "Certain-full-normalization." By this we mean that we require $<\underset{\sim}{\chi}|\underset{\sim}{\chi}> = \underset{\approx}{1}$ (where $\underset{\approx}{1}$ is the unit matrix) and we require that the phase of $\underset{\sim}{\chi}$ be determined according to equation (17) of Certain and Hirschfelder's (1970a) paper.

The prescription for recovering $\underset{\sim}{\Psi}$ and $\underset{\approx}{W}$ is this. We may recover the diagonal elements of $\underset{\approx}{W}$ as the roots to the following secular equation (the off-diagonal elements of $\underset{\approx}{W}$ are zero):

$$\det|\underset{\sim}{\chi}^{\dagger}(H_F - W)\underset{\sim}{\chi}| = 0 \qquad \text{(X-12)}$$

where in defining $\underset{\sim}{\chi}^{\dagger}$ we must take note of whether H_F is hermitian or non-hermitian.

Case (1). Let H_F be hermitian and let $\underset{\sim}{\chi} = (\Sigma_j\, C_{ja}|j\rangle, \Sigma_j\, C_{jb}|j\rangle)$ where the C_{ji}'s are expansion coefficients and the index j ranges over all members of a basis set which spans H_F . For this case $\underset{\sim}{\chi}^{\dagger}$ becomes:

$$\underset{\sim}{\chi}^{\dagger} = (\sum_j C^*_{ja}\langle j|, \sum_j C^*_{jb}\langle j|)^T \qquad \text{(X-12a)}$$

where "T" indicates taking a matrix transpose. Thus in this case, $\underset{\sim}{\chi}^{\dagger}$ is just the hermitian transpose of $\underset{\sim}{\chi}$.

Case (2). Let H_F be non-hermitian, and in particular, let it be given by Eq. (V-2). Let $\underset{\sim}{\chi}$ be expanded in the $(|A,j\rangle, |B,j\rangle)$ basis:

$$\underset{\sim}{\chi} = (\sum_{k=a,b}\sum_{j=-\infty}^{\infty} C_{kj}(a)|k,j\rangle, \sum_{k=a,b}\sum_{j=-\infty}^{\infty} C_{kj}(b)|k,j\rangle) \qquad \text{(X-12b)}$$

where the $C_{kj}(a)$'s and $C_{kj}(b)$'s are expansion coefficients. For the case of H_F being given by Eq. (V-2), $\underset{\sim}{\chi}^{\dagger}$ is defined by:

$$\underset{\sim}{\chi}^{\dagger} = \left(\sum_{k=a,b} \sum_{j=-\infty}^{\infty} C_{kj}(a)\langle k,j|, \sum_{k=a,b} \sum_{j=-\infty}^{\infty} C_{kj}(b)\langle k,j| \right)^{T} \qquad \text{(X-12c)}$$

where the "T" again indicates taking a matrix transpose. Note that when $\delta = 0$, Case (2) reduces to Case (1) because α and β have been defined as real.

In terms of the components of $\underset{\sim}{\chi}$, the secular equation (X-12) explicitly is:

$$\det\left| \begin{pmatrix} \langle\chi_a|H_F|\chi_a\rangle & \langle\chi_a|H_F|\chi_b\rangle \\ \langle\chi_b|H_F|\chi_a\rangle & \langle\chi_b|H_F|\chi_b\rangle \end{pmatrix} - W \begin{pmatrix} \langle\chi_a|\chi_a\rangle & \langle\chi_a|\chi_b\rangle \\ \langle\chi_b|\chi_a\rangle & \langle\chi_b|\chi_b\rangle \end{pmatrix} \right| = 0 \qquad \text{(X-13)}$$

where again we must take care in defining the matrix elements. Let H_F be given by Eq. (V-2) and let $\hat{O}$ be an operator equal to H_F <u>or</u> unity. Using the definition of $\underset{\sim}{\chi}$ given by Eq. (X-12b) we have

$$\langle\chi_\ell|\hat{O}|\chi_m\rangle = \sum_{k}\sum_{j}\sum_{k'}\sum_{j'} C_{kj}(\ell)\, C_{k'j'}(m)\langle k,j|\hat{O}|k',j'\rangle \qquad \text{(X-13a)}$$

where ℓ, m, k and k' can equal a or b and j as well as j' ranges from $-\infty$ to $+\infty$.

Call the two roots of (X-13), μ_1 and μ_2 . $\underset{\approx}{W}$ therefore is

$$\underset{\approx}{W} = \begin{pmatrix} \mu_1 & 0 \\ 0 & \mu_2 \end{pmatrix}$$

If the eigenvector associated with μ_1 is put in the first column of a 2×2 matrix and if the eigenvector associated with μ_2 is put in the second column of the same 2×2 matrix, the resulting matrix is just $\underset{\approx}{c}^{-1}$ (the inverse of the square matrix $\underset{\approx}{c}$ in (X-7)). Therefore $\underset{\sim}{\Psi}$ is recovered by:

$$\underset{\sim}{\Psi} = \underset{\sim}{\chi}\, \underset{\approx}{c}^{-1} \qquad \text{(X-14)}$$

<u>Perturbation Solution of (X-9)</u>

In what went just before, we assumed that we knew the solution to (X-9). For the sake of completeness, we showed how to unscramble (X-9) to recover the solutions to the Schrödinger equation, equation (X-4). In point of fact, (X-9) is every bit as difficult to solve as (X-4). To solve (X-9) we must use perturbation theory.

Assume that H_F has been broken up according to the field strength expansion:

$$H_F = H_F^{(0)} + \lambda H_F^{(1)} \qquad \text{(X-15)}$$

where $H_F^{(0)}$ is defined in terms of the $|k,j\rangle$ basis by (VII-2) and $H_F^{(1)}$ is defined in terms of the same basis by (VII-3). λ is an ordering parameter.

We will further assume that <u>both</u> $\underset{\sim}{\chi}$ <u>and</u> $\underset{\approx}{E}$ may be expanded in powers of λ :

$$\underset{\sim}{\chi} = \sum_{n=0}^{\infty} \lambda^n \underset{\sim}{\chi}^{(n)} \; ; \quad \underset{\approx}{E} = \sum_{n=0}^{\infty} \lambda^n \underset{\approx}{E}^{(n)} \tag{X-16}$$

The $\underset{\sim}{\chi}^{(n)}$'s are 1×2 row vectors and the $\underset{\approx}{E}^{(n)}$'s are 2×2 matrices.

After substituting the expansions (X-15) and (X-16) into (X-9), we may group terms in like powers of λ to get the following solvable set of matrix perturbation equations:

$$H_F^{(0)} \underset{\sim}{\chi}^{(0)} = \underset{\sim}{\chi}^{(0)} \underset{\approx}{E}^{(0)} \tag{X-17}$$

$$H_F^{(0)} \underset{\sim}{\chi}^{(1)} + H_F^{(1)} \underset{\sim}{\chi}^{(0)} = \underset{\sim}{\chi}^{(0)} \underset{\approx}{E}^{(1)} + \underset{\sim}{\chi}^{(1)} \underset{\approx}{E}^{(0)} \tag{X-18}$$

$$H_F^{(0)} \underset{\sim}{\chi}^{(2)} + H_F^{(1)} \underset{\sim}{\chi}^{(1)} = \underset{\sim}{\chi}^{(0)} \underset{\approx}{E}^{(2)} + \underset{\sim}{\chi}^{(1)} \underset{\approx}{E}^{(1)} + \underset{\sim}{\chi}^{(2)} \underset{\approx}{E}^{(0)} \tag{X-19}$$

. . . . etc.

If the zeroth order states $|k_1,n_1>$ and $|k_0,n_0>$ are almost (or exactly) degenerate, we would choose

$$\underset{\sim}{\chi}^{(0)} = (|k_1,n_1> \; , \; |k_0,n_0>) \tag{X-20}$$

and, therefore,

$$\underset{\approx}{E}^{(0)} = \begin{pmatrix} \mu_{k_1,n_1}^{(0)} & 0 \\ 0 & \mu_{k_0,n_0}^{(0)} \end{pmatrix}$$

where $\mu^{(0)}_{k_1,n_1}$ is the zeroth order energy associated with $|k_1,n_1\rangle$ and $\mu^{(0)}_{k_0,n_0}$ is the zeroth order energy associated with the state $|k_0,n_0\rangle$. The perturbation equations can be solved order-by-order if we choose "intermediate" normalization which is defined by:

$$\langle\chi_i^{(0)}|\chi_j^{(n)}\rangle = \delta_{n0}\,\delta_{ij}$$

where i,j = a or b and δ_{n0} and δ_{ij} are Kröneckar deltas. The important point in this perturbation theory is, however, that it, unlike the Rayleigh-Schrödinger treatment, allows us to avoid bad denominators of the form

$$\mu^{(0)}_{k_1,n_1} - {}^{(0)}_{k_0,n_0}$$

in the higher order wavefunctions and energies.

Introduction of some new notation is in order at this point. Assume that we know $\underset{\sim}{\chi}^{(0)}, \underset{\sim}{\chi}^{(1)}, \underset{\sim}{\chi}^{(2)}, \ldots, \underset{\sim}{\chi}^{(N)}$. Let us define the partial sum, $\underset{\sim}{\chi}(N)$, by:

$$\underset{\sim}{\chi}(N) = \sum_{n=0}^{N} \lambda^n \underset{\sim}{\chi}^{(n)} \tag{X-21}$$

We can make analogous definitions for the components of $\underset{\sim}{\chi}$:

$$|\chi_a(N)\rangle = \sum_{n=0}^{N} \lambda^n |\chi_a^{(n)}\rangle \; ; \quad |\chi_b(N)\rangle = \sum_{n=0}^{N} \lambda^n |\chi_b^{(n)}\rangle \qquad \text{(X-22)}$$

If we have solved the first (N+1) perturbation equations so that we know $\underset{\sim}{\chi}(N)$, we may recover approximations to two eigenvalues and two eigenvectors of H_F by forming the approximate secular equation:

$$\det \left| \begin{pmatrix} \langle\chi_a(N)|H_F|\chi_a(N)\rangle & \langle\chi_a(N)|H_F|\chi_b(N)\rangle \\ \langle\chi_b(N)|H_F|\chi_a(N)\rangle & \langle\chi_b(N)|H_F|\chi_b(N)\rangle \end{pmatrix} - W \begin{pmatrix} \langle\chi_a(N)|\chi_a(N)\rangle & \langle\chi_a(N)|\chi_b(N)\rangle \\ \langle\chi_b(N)|\chi_a(N)\rangle & \langle\chi_b(N)|\chi_b(N)\rangle \end{pmatrix} \right| = 0 \qquad \text{(X-23)}$$

where the above matrix elements are defined in analogy to Eq. (XI-13a). We call (X-23) an "approximate" secular equation because its roots are approximations to the exact solutions to (X-4). We will call the two approximate roots to (X-23) $\mu_1(N)$ and $\mu_2(N)$. We will use the argument "N" on the approximate roots to indicate that they arise from a secular equation in which the $\underset{\sim}{\chi}$ is accurate through N-th order. The roots themselves are accurate through (2N+1)-th order.

Associated with the approximate root, $\mu_j(N)$ $(j = 1,2)$, is an approximate wavefunction. Call this approximate wavefunctions $|\mu_j(N)\rangle$. We can obtain $|\mu_j(N)\rangle$ from the secular equation (X-23) in the following manner. Associated with the root $\mu_j(N)$ is the eigenvector*:

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* The odd-looking notation for the vector-components is chosen to keep this discussion in accord with equation (X-14).

$$\begin{pmatrix} c(N)^{-1}_{j1} \\ c(N)^{-1}_{j2} \end{pmatrix}$$

With this eigenvector we can recover the approximate wavefunction associated with $\mu_j(N)$ by the following relationship:

$$|\mu_j(N)\rangle \;=\; c(N)^{-1}_{j1}|\chi_a(N)\rangle + c(N)^{-1}_{j2}|\chi_b(N)\rangle \qquad \text{(X-24)}$$

The $|\mu_j(N)\rangle$'s , however, are correct only through order λ^N .

In the partitioning, therefore, we may obtain a whole heirarchy of approximate expressions for μ and $|\mu\rangle$, depending upon the accuracy of the $\underset{\sim}{\chi}$ we use in the secular equation (X-23). If, for example, we use $\underset{\sim}{\chi}(0)$ in (X-23), we will call the resulting approximate $\mu_j(0)$'s and $|\mu_j(0)\rangle$'s the "zeroth order" partitioning approximation. $\underset{\sim}{\chi}(1)$ will give rise to the "first order" partitioning approximation, etc.

In terms of the time-dependent Floquet Normal Modes, the $\mu_j(N)$'s correspond to approximations to the Floquet characteristic exponents. The ϕ-part of the Normal Modes may be recovered from (X-24) (i.e. the eigenvector associated with the root $\mu_j(N)$) by using the equivalence between the static problem and the dynamic problem described by (V-7) and (V-8).

Convergence of the Partitioning Perturbation Theory

We intend to use partitioning to include some of the ranges of the parameters which are not covered by the cases given in (VII-13). Specifically we will use it to cover the cases in which δ, α, and $\beta \ll 1$, but $\varepsilon \approx n_r$ (where n_r is some non-zero, positive integer).

The cases in which $\varepsilon \approx n_r$ are very interesting. When $\varepsilon \approx 1$, this means that the frequency, ω, is nearly or exactly equal to the separation between energy levels, ΔW. This is, of course, the Bohr Frequency Condition (with $\hbar$ set equal to unity). Thus when $\varepsilon \approx 1$, we are describing the two-level system's Main Resonance. Finding partitioning perturbation approximations in this regime is fully discussed in Section XI of this report. The cases in which $\varepsilon \approx n_r$ where n_r is some integer greater than one, correspond to the system's Sub-Harmonic Resonances. These are more fully discussed in Section XII of this report.

If $\varepsilon \approx n_r$ and δ is very small (or vanishing), let

$$\underset{\sim}{\chi}^{(0)} = (|A,j_0\rangle\ ,\ |B,j_0-n_r\rangle) \qquad \text{(X-25)}$$

$$j_0 \text{ any integer or zero}$$

We have made this choice because

$$\mu^{(0)}_{A,j_0} - \mu^{(0)}_{B,j_0-n_r} = (n_r - \varepsilon + i\delta) \approx 0 \qquad \text{(X-26)}$$

and with this choice, the partitioning theory enables us to avoid the occurrence of small denominators such as (X-26) in the higher order corrections to $\underset{\sim}{\chi}^{(0)}$ (and therefore in the approximate expressions for the solutions to $H_F|\mu\rangle = \mu|\mu\rangle$).

Let us assume that the components of $\underset{\sim}{\chi}$ may be expanded according to (X-22). The functions $|\chi_a^{(n)}\rangle$ and $|\chi_b^{(n)}\rangle$ may in turn be expanded in terms of the spectrum of $H_F^{(0)}$ in this manner:

$$|\chi_a^{(n)}\rangle = \sum_{\ell=A,B}{}' \sum_{m=-\infty}^{\infty}{}' g_{\ell,m}^{(n)}|\ell,m\rangle$$

$$|\chi_b^{(n)}\rangle = \sum_{\ell=A,B}{}' \sum_{m=-\infty}^{\infty}{}' d_{\ell,m}^{(n)}|\ell,m\rangle \qquad \text{(X-27)}$$

where the $g_{\ell,m}^{(n)}$'s and the $d_{\ell,m}^{(n)}$'s are the expansion coefficients and the primes on the summation signs mean that the states $|A,j_0\rangle$ and $|B,j_0-n_r\rangle$ are to be excluded from the sums. The important thing we wish to stress is that the $g_{\ell,m}^{(n)}$'s and $d_{\ell,m}^{(n)}$'s may be expressed as products of terms of the form

$$G = \frac{\langle k,n|H_F^{(1)}|k',n'\rangle}{\mu_{k,n}^{(0)} - \mu_{k_0,n_0}^{(0)}} \qquad \text{(X-28)}$$

The $\mu_{\ell,m}^{(0)}$'s are eigenvalues of $H_F^{(0)}$:

$$H_F^{(0)}|\ell,m\rangle = \mu_{\ell,m}^{(0)}|\ell,m\rangle \ .$$

(X-28) differs from a similar expression which we used to discuss the convergence of the non-degenerate Rayleigh-Schrödinger perturbation series (i.e., expression (VII-8)) only by the restrictions placed on the indices. In (X-28), if $k_0 = A$, then n_0 can only equal j_0. If $k_0 = B$, then n_0 can only equal $(j_0 - n_r)$. If $k = k_0$ then n may not equal n_0. If $k_0 = A$, then n may not equal $(j_0 - n_r)$. Similarly, if $k_0 = B$, then n may not equal j_0. Otherwise, k and k' may be either A or B. n and n' can equal any integer from $-\infty$ to $+\infty$.

If all terms of the form of G are small, we would expect that the partitioning perturbation expressions for the $\mu(N)$'s and $|\mu(N)\rangle$'s would be quickly converging.

From the definition of $H_F^{(1)}$ in (VII-3), the numerator of G can be either α, β or zero.

In considering the denominator of G, we will look at the following three cases:

Case 1: $k = k_0 = A$ or B.

If $k = k_0 = A$ or B, the denominator of G is always some non-zero integer. In this case the smallest magnitude of the denominator is unity. For terms of the form G to be much smaller than unity we require:

both α and β should be much less than unity.

<u>Case 2: $k \neq k_0 = A$; $\delta << 1$.</u>

In this case, the denominator of G is of the form

$$(n + \varepsilon - i\delta - j_0) \ . \qquad \text{(X-29)}$$

Since n can never equal $(j_0 - n_r)$, (X-29) is of the form

$$(m - i\delta)$$

where m is some (positive or negative) non-zero integer. Clearly, since $\delta << 1$, $(m - i\delta)$ is of order unity or larger. Thus we get no additional requirements for the speedy convergence of the partitioning perturbation series.

<u>Case 3: $k \neq k_0 = B$; $\delta << 1$.</u>

The arguments and conclusions in this case are the same as those we used in discussing Case 2.

We may therefore summarize and conclude this discussion by saying: <u>If $\varepsilon \approx n_r$ where n_r is a positive non-zero integer and, if α, β and δ are all much less than unity, we may use partitioning perturbation theory to obtain rapidly converging field-strength perturbation solutions to $H_F|\mu\rangle = \mu|\mu\rangle$</u>.

XI. TECHNIQUE T6: PARTITIONING PERTURBATION THEORY APPLIED TO THE MAIN RESONANCE: $\varepsilon \approx 1$. α β AND δ ARE ALL MUCH LESS THAN UNITY

Introduction

In this section we will discuss the solutions to

$$H_F|\mu> \quad = \quad \mu|\mu> \qquad \text{(XI-1)}$$

under the conditions that $\varepsilon \simeq 1$ and α, β and δ are all much less than unity. In terms of the non-reduced parameters, this, of course, means that $\omega \approx \Delta W$. The conditions are therefore the conditions under which the Bohr Frequency condition is met: $(W_b - W_a) = \hbar\omega$.

To separate this regime of $\varepsilon \simeq 1$ from the regime of $\varepsilon \approx n_r$ where n_r is some positive integer greater than unity, is somewhat artificial. Partitioning pertubation theory is used to handle both regimes. The separation is justified, however because of the great amount of previous work devoted to the case of $\varepsilon \approx 1$.

We split this section up into two parts. In the first part we use partitioning perturbation theory to obtain systematic, converging approximations to the eigenvalue-eigenvector problem given by (XI-1). Once (XI-1) is solved, we can recover the time-dependent solutions to (II-4) and (II-5) by utilizing the equivalence between the static and dynamic problems which we have already established. Our method of solution closely parallels that of Shirley (1965). We differ from Shirley in not restricting our attention to the special case of $V_{aa} = V_{bb} = \gamma_a = \gamma_b = 0$. Furthermore, Shirley uses a partitioning scheme formulated by Salwen (1955) in which the higher order corrections to $\underset{\sim}{\chi}^{(0)}$ are only approximately found whereas we obtain exact solutions for the higher order corrections to $\underset{\sim}{\chi}^{(0)}$.

In the second part we discuss how our work fits in with the work previously done on the main resonance of the two-level system. We find that the partitioning perturbation theory is a useful tool for relating and comparing our work with that of Rabi (1937), Bloch and Siegert (1940), Stevenson (1940), Shirley (1965), Silverman and Pipkin (1972), Winter (1959) and Pegg (1973b).

Part I: Partitioning Perturbation Solutions When $\varepsilon \simeq 1$. α, β and δ Are All Much Less Than Unity.

When $\varepsilon \simeq 1$ and $\delta << 1$, the kets $|A,j_0\rangle$ and $|B,j_0-1\rangle$ are almost degenerate with respect to $H_F^{(0)}$ when j_0 is either zero or any positive or negative integer. In order to avoid perturbation denominators of the form $(\varepsilon - 1 + i\delta)$ which result from this almost degeneracy, we use partitioning perturbation techniques. First, H_F is split into a zeroth order part which is independent of the field strength and a first order perturbation proportional to the field strength. Then we choose $\underset{\sim}{\chi}^{(0)}$ to be the two-component row vector:

$$\underset{\sim}{\chi}^{(0)} = (|A,j_0\rangle, |B,j_0-1\rangle) \tag{XI-2}$$

where j_0 is any integer or zero.

Since the final time-dependent results for the characteristic exponents and the Fourier components do not depend on the choice of j_0 , we will for the sake of simplicity choose $j_0 = 0$. Therefore let

$$\underset{\sim}{\chi}^{(0)} = (|A,0\rangle, |B,-1\rangle) \tag{XI-3}$$

The Zeroth Order Partitioning Approximation

Since we have chosen $\underset{\sim}{\chi}^{(0)}$ by (XI-3), we may now obtain the zeroth order partitioning approximation. This involves solving the secular equation (X-23) with $N = 0$. By definition,

$$\underset{\sim}{\chi}(0) = \underset{\sim}{\chi}^{(0)} . \tag{XI-4}$$

With this expression we may explicitly write the zeroth order secular equation:

$$\det\begin{vmatrix} -W & \alpha \\ \alpha & (\varepsilon-1-i\delta)-W \end{vmatrix} = 0 \tag{XI-5}$$

In writing the zeroth order secular equation we have set the ordering parameter, λ , equal to unity.

There are two roots to (XI-5), $\mu_1(0)$ and $\mu_2(0)$, which correspond to approximations to the Floquet characteristic exponents accurate through first order in the field strength. The roots are explicitly given by:

$$\mu_1(0) = \tfrac{1}{2}[(\varepsilon - 1 - i\delta) - \{(\varepsilon - 1 - i\delta)^2 + 4\alpha^2\}^{1/2}] \qquad \text{(XI-6)}$$

$$\mu_2(0) = \tfrac{1}{2}[(\varepsilon - 1 - i\delta) + \{(\varepsilon - 1 - i\delta)^2 + 4\alpha^2\}^{1/2}] \qquad \text{(XI-7)}$$

Using the notation already defined in section X, we may write the eigenvector associated with $\mu_1(0)$ as:

$$\begin{pmatrix} 1 \\ \mu_1(0)/\alpha \end{pmatrix} = \begin{pmatrix} c(0)^{-1}_{11} \\ c(0)^{-1}_{21} \end{pmatrix} \qquad \text{(XI-8)}$$

Associated with the root $\mu_2(0)$ is the eigenvector:

$$\begin{pmatrix} \alpha/\mu_2(0) \\ 1 \end{pmatrix} = \begin{pmatrix} c(0)^{-1}_{12} \\ c(0)^{-1}_{22} \end{pmatrix} \qquad \text{(XI-9)}$$

Using (X-24) and (XI-8), we may write the approximate wavefunction associated with the approximate root $\mu_1(0)$ as:

$$|\mu_1(0)\rangle = |A,0\rangle + \frac{\mu_1(0)}{\alpha}|B,-1\rangle \qquad \text{(XI-10)}$$

Associated with the approximate root $\mu_2(0)$ is:

$$|\mu_2(0)\rangle = \frac{\alpha}{\mu_2(0)}|A,0\rangle + |B,-1\rangle \qquad \text{(XI-11)}$$

With these approximate energies and wavefunctions, we can use the equivalence between the static and dynamic problems to obtain the "zeroth order" partitioning approximation for the two time-dependent Floquet Normal Modes:

First Mode

$$\mu_1(0) = \tfrac{1}{2}[(\varepsilon - 1 - i\delta) - \{(\varepsilon - 1 - i\delta)^2 + 4\alpha^2\}^{1/2}]$$

$$\begin{aligned} a_1 &= e^{-i\mu_1(0)\tau}\,\phi_{a1}\ ; \quad \phi_{a1} = 1 \\ b_1 &= e^{-i\mu_1(0)\tau}\,\phi_{b1}\ ; \quad \phi_{b1} = \left(\frac{\mu_1(0)}{\alpha}\right)e^{-i\tau} \end{aligned} \qquad \text{(XI-12)}$$

Second Mode

$$\mu_2(0) = \tfrac{1}{2}[(\varepsilon - 1 - i\delta) + \{(\varepsilon - 1 - i\delta)^2 + 4\alpha^2\}^{1/2}]$$

$$\begin{aligned} a_2 &= e^{-i\mu_2(0)\tau}\,\phi_{a2}\ ; \quad \phi_{a2} = \alpha/\mu_2(0) \\ b_2 &= e^{-i\mu_2(0)\tau}\,\phi_{b2}\ ; \quad \phi_{b2} = e^{-i\tau} \end{aligned} \qquad \text{(XI-13)}$$

Again we wish to note that in these "zeroth order" expressions for the Floquet solutions the characteristic exponents are accurate through first order in the field strength whereas the "ϕ-parts" of the Floquet Modes are accurate only through zeroth order in F. It is also interesting to note that the parameter β does not appear in this zeroth order approximation. It does, however, appear in the higher order partitioning approximations.

The First Order Partitioning Approximation

We may obtain more accurate results for the Floquet Normal Modes by using the "first order" partitioning approximation. By this we mean that we find an expression for the row vector $\underset{\sim}{\chi}$ which is correct through first order in the field strength, i.e. we determine $\underset{\sim}{\chi}(1)$. This $\underset{\sim}{\chi}(1)$ is then used in the secular equation, (X-23). The resulting secular equation may be solved to obtain two roots, $\mu_1(1)$ and $\mu_2(1)$, which correspond to approximations to the Floquet characteristic exponents which are accurate through third order in F. The approximate eigenfunctions, $|\mu_1(1)\rangle$ and $|\mu_2(1)\rangle$, which are related to $\mu_1(1)$ and $\mu_2(1)$ respectively may be used to obtain the "ϕ-parts" to the Floquet Normal Modes which are correct through first order in F.

We have already chosen

$$\underset{\sim}{\chi}^{(0)} = (|A,0\rangle, |B,-1\rangle) . \qquad \text{(XI-14)}$$

In order that the zeroth order perturbation equation

$$H^{(0)} \underset{\sim}{\chi}^{(0)} = \underset{\sim}{\chi}^{(0)} \underset{\approx}{E}^{(0)}$$

be satisfied, we must choose

$$\underset{\approx}{E}^{(0)} = \begin{pmatrix} 0 & 0 \\ 0 & (\varepsilon-1-i\delta) \end{pmatrix} \qquad \text{(XI-15)}$$

$\underset{\sim}{\chi}^{(1)}$ obeys the equation:

$$H^{(0)} \underset{\sim}{\chi}^{(1)} + H^{(1)} \underset{\sim}{\chi}^{(0)} = \underset{\sim}{\chi}^{(1)} \underset{\approx}{E}^{(0)} + \underset{\sim}{\chi}^{(0)} \underset{\approx}{E}^{(1)} \qquad \text{(XI-16)}$$

In solving (XI-16), we must specify the normalization of $\underset{\sim}{\chi}^{(1)}$.
We will choose "intermediate normalization":

$$\langle k,\ell|\chi_j^{(1)}\rangle = 0 \ ; \quad j = a \text{ or } b \ ; \quad (k,\ell) = (A,0) \text{ or } (B,-1) \qquad \text{(XI-17)}$$

Substituting

$$\underset{\sim}{\chi}^{(1)} = (|\chi_a^{(1)}\rangle, |\chi_b^{(1)}\rangle)$$

into Eq. (XI-16), we obtain the following equations for $|\chi_a^{(1)}\rangle$ and $|\chi_b^{(1)}\rangle$:

$$H^{(0)}|\chi_a^{(1)}\rangle + H^{(1)}|A,0\rangle = (\underset{\approx}{E}^{(1)})_{11}|A,0\rangle + (\underset{\approx}{E}^{(1)})_{21}|B,-1\rangle \tag{XI-18}$$

$$[H^{(0)} - \varepsilon + 1 + i\delta]|\chi_b^{(1)}\rangle + H^{(1)}|B,-1\rangle = (\underset{\approx}{E}^{(1)})_{12}|A,0\rangle + (\underset{\approx}{E}^{(1)})_{22}|B,-1\rangle \tag{XI-19}$$

To fulfill the normalization condition in Eq. (XI-17), we let

$$|\chi_a^{(1)}\rangle = \sum_{\ell=A,B}\sum_{m=-\infty}^{\infty} g_{\ell,m}^{(1)}(1 - \delta_{\ell,A}\delta_{m,0})(1 - \delta_{\ell,B}\delta_{m,-1})|\ell,m\rangle \tag{XI-20}$$

$$|\chi_b^{(1)}\rangle = \sum_{\ell=A,B}\sum_{m=-\infty}^{\infty} d_{\ell,m}^{(1)}(1 - \delta_{\ell,A}\delta_{m,0})(1 - \delta_{\ell,B}\delta_{m,-1})|\ell,m\rangle \tag{XI-21}$$

where the $g_{\ell,m}^{(1)}$'s and $d_{\ell,m}^{(n)}$'s are expansion coefficients and the $\delta_{i,j}$'s are Krönecker "deltas." Substituting the expansions (XI-20) and (XI-21) into Eqs. (XI-18) and (XI-19), we multiply the resulting equations first by $\langle A,0|$ and then by $\langle B,-1|$ to find:

$$(\underset{\approx}{E}^{(1)})_{ij} = \alpha(\delta_{ij} - 1)$$

where δ_{ij} is the Krönecker "delta." In a similar manner we find:

$$|\chi_a^{(1)}\rangle = \frac{-\alpha}{(\varepsilon + 1 - i\delta)} |B,1\rangle$$

$$|\chi_b^{(1)}\rangle = \beta(|B,-2\rangle - |B,0\rangle) + \frac{\alpha}{(\varepsilon + 1 - i\delta)} |A,-2\rangle \qquad \text{(XI-22)}$$

Setting λ equal to unity $\underset{\sim}{\chi}(1)$ is simply

$$\underset{\sim}{\chi}(1) = \underset{\sim}{\chi}^{(0)} + \underset{\sim}{\chi}^{(1)}$$

where $\underset{\sim}{\chi}^{(0)}$ is given by (XI-14) and $\underset{\sim}{\chi}^{(1)}$ is given by (XI-22).

We may now form the first order secular equation by using $\underset{\sim}{\chi}(1)$ in (X-23) to obtain:

$$\det\left|\begin{pmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{pmatrix} - \mu\begin{pmatrix} s_{11} & 0 \\ 0 & s_{22} \end{pmatrix}\right| = 0 \qquad \text{(XI-23)}$$

where λ has been set equal to unity and where:

$$h_{11} = -\alpha^2/(\varepsilon + 1 - i\delta)$$

$$h_{12} = h_{21} = \alpha + \alpha\beta^2/(\varepsilon + 1 - i\delta)$$

$$h_{22} = (\varepsilon - 1 - i\delta)(1 + 2\beta^2) + 2\alpha^2(\varepsilon - i\delta)/(\varepsilon + 1 - i\delta)^2 \qquad \text{(XI-24)}$$

$$s_{11} = 1 + \alpha^2/(\varepsilon + 1 - i\delta)^2$$

$$s_{22} = 1 + 2\beta^2 + \alpha^2/(\varepsilon + 1 - i\delta)^2$$

Just as we did in discussing the zeroth order partitioning approximation, we may use the j-th root of (XI-23), $\mu j(1)$ $(j = 1,2)$, and its associated eigenvector

$$\begin{pmatrix} c(1)^{-1}_{1j} \\ \\ c(1)^{-1}_{2j} \end{pmatrix}$$

to obtain approximate expressions for the time-dependent Floquet Normal Modes.

First Mode:

$$a_1 = e^{-i\mu_1(1)\tau}\,\phi_{a1}\;; \qquad b_1 = e^{-i\mu_1(1)\tau}\,\phi_{b1}$$

$$\mu_1(1) = \tfrac{1}{2}\Big[\frac{h_{22}}{s_{22}} + \frac{h_{11}}{s_{11}} - \Big[\Big(\frac{h_{22}}{s_{22}} + \frac{h_{11}}{s_{11}}\Big)^2 - 4\Big(\frac{h_{11}h_{22} - (h_{12})^2}{s_{11}s_{22}}\Big)\Big]^{1/2}\Big]$$

$$c(1)^{-1}_{21} = \frac{h_{12}}{(s_{11}\mu_1(1) - h_{11})} \qquad \text{(XI-25)}$$

$$\phi_{a1} = 1 + \frac{\alpha c(1)^{-1}_{21}\, e^{-2i\tau}}{(\varepsilon + 1 - i\delta)}$$

$$\phi_{b1} = \frac{-\alpha\, e^{i\tau}}{(\varepsilon + 1 - i\delta)} + c(1)^{-1}_{21}[e^{-i\tau} + \beta(e^{-2i\tau} - 1)]$$

Second Mode:

$$a_2 = e^{-i\mu_2(1)\tau}\,\phi_{a2}\;; \qquad b_2 = e^{-i\mu_2(1)\tau}\,\phi_{b2}$$

$$\mu_2(1) = \tfrac{1}{2}\Big[\frac{h_{22}}{s_{22}} + \frac{h_{11}}{s_{11}} + \Big[\Big(\frac{h_{22}}{s_{22}} + \frac{h_{11}}{s_{11}}\Big)^2 - 4\Big(\frac{h_{11}h_{22} - (h_{12})^2}{s_{11}s_{22}}\Big)\Big]^{1/2}\Big]$$

$$c(1)^{-1}_{12} = \frac{h_{12}}{\mu_2(1)s_{11} - h_{11}} \qquad \text{(XI-26)}$$

$$\phi_{a2} = c(1)^{-1}_{12} + \frac{\alpha\, e^{-2i\tau}}{(\varepsilon + 1 - i\delta)}$$

$$\phi_{b1} = e^{-i\tau} + \beta(e^{-2i\tau} - 1) - \frac{c(1)^{-1}_{12}\, \alpha e^{i\tau}}{(\varepsilon + 1 - i\delta)}$$

The s_{ij}'s and h_{ij}'s which appear in (XI-25) and (XI-26) have already been defined in terms of the fundamental parameters of the problem by the expressions in (XI-24).

The Second Order Partitioning Approximation

We may use partitioning to obtain still better approximations. For example, we may form the second order correction to $\underset{\sim}{\chi}$,

$$\underset{\sim}{\chi}^{(2)} = (|\underset{\sim}{\chi}_a^{(2)}>, |\underset{\sim}{\chi}_b^{(2)}>).$$

This function is found by solving (X-19). If we impose intermediate normalization

$$<k,\ell|\chi_j^{(2)}> = 0 \ ; \quad j = a \text{ or } b \ ; \quad (k,\ell) = (A,0) \text{ or } (B,-1)$$

we find the following results for $|\chi_a^{(2)}>$ and $|\chi_b^{(2)}>$:

$$|\chi_a^{(2)}> = \frac{\alpha^2}{2(\varepsilon + 1 - i\delta)} [|A,2> - |A,-2>] - \frac{\alpha\beta}{(\varepsilon + 1 - i\delta)} |B,0> + \frac{\alpha\beta}{(\varepsilon - 2 - i\delta)} |B,-2> + \frac{\alpha\beta|B,2>}{(\varepsilon + 1 - i\delta)(\varepsilon + 2 - i\delta)}$$

(XI-27)

$$|\chi_b^{(2)}> = \frac{\alpha\beta}{(\varepsilon + 2 - i\delta)} |A,-3> - \frac{\alpha\beta|A,1>}{(\varepsilon - 2 - i\delta)} + (\frac{\beta^2}{2} + \frac{\alpha^2}{2(\varepsilon + 1 - i\delta)})|B,-3> + (\frac{\beta^2}{2} - \frac{\alpha^2}{2(\varepsilon + 1 - i\delta)})|B,1>$$

Using (XI-3), (XI-22) and (XI-27), we may form $\underset{\sim}{\chi}(2)$. This $\underset{\sim}{\chi}(2)$ is correct through second order in λ and it may be used to form the second order partitioning secular equation, i.e. equation (X-23) with $N = 2$. We will obtain from this secular equations two roots correct through fifth order in F . These roots correspond to the Floquet characteristic exponents. We will also obtain two approximate wavefunctions, $|\mu_j(2)\rangle \; j = 1,2$, which will be correct through second order in F . These will correspond to the "ϕ-parts" of the Floquet Normal Modes. The explicit results of the second order partitioning approximation are not given since they are algebraically cumbersome.

Part II: Relationship of Partitioning Perturbation Solutions to Other Solutions. $\varepsilon \approx 1$.

Since the regime of $\varepsilon \approx 1$ is of great spectroscopic interest, many authors have considered the two-level system at its main resonance. Since the problem is usually considered with $\beta = \delta = 0$, we will first discuss the solutions under the conditions that $\beta = \delta = 0$.

Textbook Solutions: $\beta = \delta = 0$

If we set β and δ equal to zero, equations (II-4) and (II-5) become

$$\begin{aligned} \dot{a} &= -2i\alpha \cos\tau \; b \\ \dot{b} &= -i\varepsilon b - 2i\alpha \cos\tau \; a \end{aligned} \qquad \text{(XI-28)}$$

The usual textbook* solution to (XI-28) proceeds in the following manner. First transform (XI-28) by letting

$$b(\tau) = b'(\tau)e^{-i\tau}$$

The equations for $b'(\tau)$ and $a(\tau)$ therefore become:

$$\begin{aligned} \dot{a}(\tau) &= -i\alpha(1 + e^{-2i\tau})b'(\tau) \\ \dot{b}'(\tau) &= -i(\varepsilon - 1)b'(\tau) - i\alpha(e^{2i\tau} + 1)a(\tau) \end{aligned} \qquad \text{(XI-29)}$$

The prescription is to now neglect all of the time-dependent coefficients in (XI-29) to obtain an easily soluable system of two linear coupled homogeneous differential equations with constant coefficients. The justification of this prescription is that the $(e^{\pm 2i\tau})$ terms are negligible because they are quickly oscillating and therefore average out to zero. There are two linearly independent solutions obtained by this prescription and they are:

$$\begin{aligned} a_1 &= \exp[-\frac{i}{2}[(\varepsilon - 1) - \{(\varepsilon - 1)^2 + 4\alpha^2\}^{1/2}\tau]] \\ b_1 &= \frac{1}{2\alpha}[(\varepsilon - 1) - \{(\varepsilon - 1)^2 + 4\alpha^2\}^{1/2}]a_1e^{-i\tau} \end{aligned} \qquad \text{(XI-30)}$$

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* See, for example, L. D. Landau and E. M. Lifshitz (1965), p. 139.

$$a_2 = \frac{2\alpha\ e^{i\tau}\ b_2}{[(\varepsilon - 1) + [(\varepsilon - 1)^2 + 4\alpha^2]^{1/2}]}$$

$$b_2 = e^{-i\tau} \exp[-\tfrac{i}{2}[(\varepsilon - 1) + \{(\varepsilon - 1)^2 + 4\alpha^2\}^{1/2}\tau]] \qquad \text{(XI-31)}$$

By inspection we can see that (XI-30) is the same as expression (XI-12) if, in (XI-12), we set δ equal to zero wherever it appears. Similarly, (XI-31) is equivalent to (XI-13). The "textbook" solutions are therefore just the zeroth order partitioning perturbation approximation to the Floquet Normal Modes. The partitioning theory therefore gives a justification for the ad hoc "textbook" method of solving (XI-28).

The solutions given by (XI-30) and (XI-31) are the exact solutions to the Schrödinger Equation for a spin $\frac{1}{2}$ particle in a rotating magnetic field. These exact solutions were first derived by Rabi (1937). When (XI-30) and (XI-31) are used as approximate solutions for a two-level system in an oscillating field, it is customary to call them the "Rabi Rotating Field Approximation."

Bloch-Siegert Solutions: $\beta = \delta = 0$

The first attempt to improve upon the Rabi Rotating Field Solutions was made by F. Bloch and A. Siegert (1940). Their important work led to the realization that the main resonance of a spin $\frac{1}{2}$ system (or, equivalently, of any two-level system) in an oscillating linearly polarized magnetic (or electric) field would

<u>not</u> occur at the frequency $\omega = \Delta W$ (or, $\varepsilon = 1$), but would be slightly "shifted," i.e. would occur at a frequency ω_0 such that

$$\omega_0 = \Delta W + \text{terms proportional to the field strength.}$$

In their treatment, Bloch and Siegert change the independent variable in Eqs. (XI-28) to

$$x = 2\tau + 2\pi$$

and they then derive an equation for the quotient $u(x) = a(x)/b(x)$:

$$\frac{du}{dx} = i\alpha\cos(x/2) + \frac{i\varepsilon u}{2} - i\alpha\cos(x/2)u^2 \qquad \text{(XI-32)}$$

Bloch and Siegert further assume that $u(x)$ has the following functional form

$$u(x) = \frac{e^{ix/2}[\Omega e^{i(z(x)-\rho x)} + (1/\Omega)]}{[1 - e^{i(z(x)-\rho x)}]} \qquad \text{(XI-33)}$$

where

$$\Omega = \frac{1}{2\alpha}[(1-\varepsilon) + ((1-\varepsilon)^2 + 4\alpha^2)^{1/2}]$$

$$\rho = \frac{\alpha}{2}[\Omega + \frac{1}{\Omega}]$$

and $z(x)$ is a function which is to be determined. Using Eq. (XI-33) in Eq. (XI-32) we find that z(x) is determined by a non-linear differential equation:

$$\frac{dz}{dx} = \Delta\left[-2(e^{ix} + e^{-ix}) + e^{iz}(e^{-i(1+\rho)x} - \Omega^2 e^{i(1-\rho)x}) + e^{-iz}(e^{-i(1-\rho)x} - \frac{1}{\Omega^2} e^{i(1+\rho)x})\right] \qquad \text{(XI-34)}$$

where $\Delta = \alpha^2/4\rho$.

At the main resonance, $\varepsilon \simeq 1$ and $\Delta \approx \alpha/4$. Δ is clearly a small quantity if the field strength (and, therefore, α) is small. Bloch and Siegert, consequently, use perturbation theory to solve Eq. (XI-34) after first assuming

$$z(x) = \sum_{n=0}^{\infty} \Delta^n z^{(n)} . \qquad \text{(XI-35)}$$

The zeroth order solution to Eq. (XI-34) is $z^{(0)} = c$ where c is an arbitrary constant. Choosing $z^{(0)} = 0$ we find that at $x = 0$, the zeroth order approximation to u evaluated at $x = 0$ has the value ∞ . This corresponds to the system's being in state $\psi_a(\underset{\sim}{r})$ at $x = 0$. Choosing $z^{(0)} = 0$ further gives the following zeroth order approximation for $a^*(x)a(x)$:

$$a^*(x)a(x) \simeq \frac{(1-\varepsilon)^2 + 2\alpha^2(1+\cos\rho x)}{(1-\varepsilon)^2 + 4\alpha^2} \qquad \text{(XI-36)}$$

Eq. (XI-36) corresponds to the Rabi Rotating Field approximate expression for the amplitude $a^*(x)a(x)$. Finding the higher order corrections to z(x) may, therefore, be thought of as finding corrections to the Rabi Rotating Field approximation.*

The Bloch-Siegert technique is cumbersome to work with; it makes no reference to the known Floquet Form of solution, and it lacks ease of extension to quantum systems with more than two energy levels. For these reasons, we do not recommend its use.

The Stevenson-Moulton Approach: $\beta = \delta = 0$

Soon after Bloch and Siegert's work was published, Stevenson (1940) rederived their result for the "resonant shift" using less cumbersome techniques.

Stevenson's starting point is equations (XI-28). He makes explicit use of the Floquet Theory by assuming that $a(\tau)$ and $b(\tau)$ may be written according to:

$$\begin{aligned} a(\tau) &= \phi_a(\tau)\, e^{-i\mu\tau} \\ b(\tau) &= \phi_b(\tau)\, e^{-i\mu\tau}\, e^{-i\tau} \end{aligned} \qquad \text{(XI-37)}$$

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* We wish to note that the equations for $z^{(n)}$ $(n > 0)$ are solvable only after $\exp[\pm iz(x)]$ has been expanded in the usual series expansion for the exponential:

$$\exp[\pm iz(x)] = 1 \pm iz(x) - \tfrac{1}{2}[z(x)]^2 \mp \ldots .$$

where μ is a constant and

$$\phi_i(\tau + 2\pi) = \phi_i(\tau) \qquad i = a,b \ .$$

The equations for the ϕ_i's become:

$$\begin{aligned} \dot{\phi}_a &= i\mu\phi_a - i\alpha(1 + e^{-2i\tau})\phi_b \\ \dot{\phi}_b &= i\mu\phi_b - i(\varepsilon - 1)\phi_b - i\alpha(1 + e^{2i\tau})\phi_a \end{aligned} \qquad \text{(XI-38)}$$

The technique which Stevenson recommends is one due to Moulton (1920). It is one in which the time-dependent terms in Eqs. (XI-38) are taken to be perturbations on the static terms. This is formally accomplished by replacing any α which multiplies a time-dependent term in Eqs. (XI-38) by $(\lambda\alpha)$ where λ is an ordering parameter. The quantities μ, ϕ_a and ϕ_b are expanded in powers of λ and a set of perturbation equations are derived which may be solved under the stipulations:*

$$\mu^{(n)} \text{ is constant for all } n \ .$$

$$\phi_j^{(n)}(\tau) = \phi_j^{(n)}(\tau + \pi) \ ; \quad \text{all } n; \ j = a,b \ .$$

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* Note that because of the transformations of Eqs. (XI-37) the "ϕ-parts" of the Floquet solutions have periodicity π rather than periodicity 2π .

The zeroth order solutions obtained by use of this technique are just the Rabi Rotating Field approximate solutions, i.e. Eqs. (XI-30) and (XI-31). The higher order corrections may, therefore, be thought of as corrections to the Rabi solutions. This technique differs from techniques such as Technique T2 (see Chapter VIII) in that the equations for the correction functions are inhomogeneous coupled (rather than homogeneous coupled) differential equations. The Stevenson-Moulton technique is similar to Technique T2 in that the $\mu^{(n)}$'s and the constants of integration (aside from normalization) are determined by the requirement that the ϕ_j's be properly periodic.

There is, however, a problem with the Stevenson-Moulton technique: the perturbation series is not quickly convergent. To most easily demonstrate this, we reformulate the dynamic problem of Eqs. (XI-38) as a static problem.

As we have done before, we use Floquet's theory and Fourier's Theorem to write:

$$\phi_a = \sum_{j=-\infty}^{\infty} \hat{A}_j e^{2ij\tau} ; \quad \phi_b = \sum_{j=-\infty}^{\infty} \hat{B}_j e^{2ij\tau} \quad \text{(XI-39)}$$

where $\hat{A}_j$ and $\hat{B}_j$ are constants and where we use the fact that the ϕ-functions in Eqs. (XI-38) have periodicity π rather than periodicity 2π.

Substituting expressions (XI-39) into Eqs. (XI-38), we derive static equations for μ and the Fourier expansion coefficients.

$$(2j - \mu)\hat{A}_j + \alpha\hat{B}_j + \alpha\lambda\hat{B}_{j+1} = 0$$
$$(2j + [\epsilon-1] - \mu)\hat{B}_j + \alpha\hat{A}_j + \alpha\lambda\hat{A}_{j-1} = 0 \qquad \text{(XI-40)}$$

In order to reformulate the problem posed by Eq. (XI-40) into a problem which has zeroth order solutions corresponding to the Rabi approximate solutions, we merely need to change basis by defining the coefficients P_j and Q_j :

$$P_j = \hat{A}_j + \frac{\mu_+^{(0)}}{\alpha}\hat{B}_j$$
$$Q_j = \hat{A}_j + \frac{\mu_-^{(0)}}{\alpha}\hat{B}_j \qquad \text{(XI-41)}$$

where

$$\mu_\pm^{(0)} = \tfrac{1}{2}[(\epsilon-1) \pm \sqrt{R}]$$

and

$$R = (\epsilon-1)^2 + 4\alpha^2$$

From Eq. (XI-41) we write:

$$\hat{A}_j = \frac{\mu_+^{(0)}}{\sqrt{R}} Q_j - \frac{\mu_-^{(0)}}{\sqrt{R}} P_j$$
$$\hat{B}_j = \frac{\alpha}{\sqrt{R}} (P_j - Q_j) \qquad \text{(XI-42)}$$

Using these definitions and using Eqs. (XI-40), we find the equations for P_j and Q_j :

$$(2j + \mu_+^{(0)} - \mu)P_j + \frac{\lambda\mu_+^{(0)}}{\sqrt{R}}(\mu_+^{(0)}Q_{j-1} - \mu_-^{(0)}P_{j-1}) + \frac{\lambda\alpha^2}{\sqrt{R}}(P_{j+1} - Q_{j+1}) = 0 \tag{XI-43}$$

$$(2j + \mu_-^{(0)} - \mu)Q_j + \frac{\lambda\alpha^2}{\sqrt{R}}(P_{j+1} - Q_{j+1}) + \frac{\lambda\mu_-^{(0)}}{\sqrt{R}}(\mu_+^{(0)}Q_{j-1} - \mu_-^{(0)}P_{j-1}) = 0 \tag{XI-44}$$

In exact analogy to what we did in Chapter V, we reformulate Eqs. (XI-43) and (XI-44) into the Schrödinger-like problem:

$$H_s|\mu\rangle = \mu|\mu\rangle \tag{XI-45}$$

where H_s is an operator, μ is an eigenvalue and $|\mu\rangle$ is a function which may be expressed in an orthonormal basis composed of all the $|P,j\rangle$'s and $|Q,j\rangle$'s :

$$\langle k,\ell|m,n\rangle = \delta_{k,m}\,\delta_{\ell,m}$$

where $k,\ell = P$ or Q and j is any integer including zero. H_s is written as

$$H_s = H_s^{(0)} + \lambda H_s^{(1)} \tag{XI-46}$$

where

$$H_s^{(0)}|P,j\rangle = (2j + \mu_+^{(0)})|P,j\rangle$$
$$H_s^{(0)}|Q,j\rangle = (2j + \mu_-^{(0)})|Q,j\rangle \qquad \text{(XI-47)}$$

and

$$H_s^{(1)}|P,j\rangle = \frac{\mu_+^{(0)}}{\sqrt{R}}(\mu_+^{(0)}|Q,j-1\rangle - \mu_-^{(0)}|P,j-1\rangle) + \frac{\alpha^2}{\sqrt{R}}(|P,j+1\rangle - |Q,j+1\rangle) \qquad \text{(XI-48)}$$

$$H_s^{(1)}|Q,j\rangle = \frac{\alpha^2}{\sqrt{R}}(|P,j+1\rangle - |Q,j+1\rangle) + \frac{\mu_-^{(0)}}{\sqrt{R}}(\mu_+^{(0)}|Q,j-1\rangle - \mu_-^{(0)}|P,j-1\rangle) \qquad \text{(XI-49)}$$

We recover the solution to the dynamic problem of Eqs. (XI-38) from the solution to the Schrödinger-type problem of Eq. (XI-45) by the following prescription. Assume we know $|\mu\rangle$ and μ . In particular, assume we know $|\mu\rangle$ as:

$$|\mu\rangle = \sum_{i=P,Q} \sum_{j=-\infty}^{\infty} c_{i,j}|i,j\rangle \qquad \text{(XI-50)}$$

where the $c_{i,j}$'s are expansion coefficients. P_j is equal to the coefficient of $|P,j\rangle$ in the expansion (XI-50). Q_j is equal to the coefficient of $|Q,j\rangle$. $\hat{A}_j$ and $\hat{B}_j$ are found by Eqs. (XI-42) once P_j and Q_j are known. Knowing $\hat{A}_j$, $\hat{B}_j$ and μ , we have completely solved the original equations, Eq. (XI-38).

The Stevenson-Moulton method is equivalent to solving Eq. (XI-45) by using Rayleigh-Schrödinger non-degenerate perturbation theory and considering the term $H_s^{(1)}$ to be the perturbation on $H_s^{(0)}$. We first seek the solution which corresponds to

$$\lim_{\lambda \to 0} \mu = \mu_+^{(0)} \; ; \quad \lim_{\lambda \to 0} |\mu> = |P,0>$$

since, in zeroth order, this solution leads to one of the Rabi approximate solutions. The other Rabi approximate solution is the zeroth order solution to Eq. (XI-45) which is defined by:

$$\lim_{\lambda \to 0} \mu = \mu_-^{(0)} \; ; \quad \lim_{\lambda \to 0} |\mu> = |Q,0> .$$

From the discussion of Chapter VII, we know that the higher order corrections in the Rayleigh-Schrödinger non-degenerate perturbation theory will contain terms of the form given by Eq. (VII-8). For the Hamiltonian $H_s^{(0)}$, the smallest difference between zeroth order energies is $\pm\sqrt{R}$ and when ε is very nearly unity,

$$\pm\sqrt{R} \simeq \pm 2\alpha .$$

When $\varepsilon \simeq 1$, <u>all</u> the matrix elements of $H_s^{(1)}$ are of order of magnitude α. Thus, some of the correction terms obtained by this method may be of order unity--the same order of magnitude of the zeroth order solutions. Thus, we do not expect the Stevenson-Moulton technique to give a quickly converging series approximation to the original problem.

Shirley's Approach: $\beta = \delta = 0$

Our technique of solving (XI-28) by using Floquet Theory and Fourier's Theorem to reduce the time-dependent problem to a time-independent eigenvalue-eigenvector problem, has been taken from Shirley's (1963,1965) work. Shirley reduces (XI-28) to the problem of solving

$$H_F|\mu\rangle = \mu|\mu\rangle$$

in the $|A,j\rangle$, $|B,j\rangle$ basis. Since he considers only the case of $\beta = \delta = 0$, H_F would be defined by (V-2) in which both δ and β have been set equal to zero. For the case of $\varepsilon \approx 1$, Shirley takes note of the fact that standard Rayleigh-Schrödinger perturbation theory may not be used to obtain quickly converging approximations. To handle this case, Shirley uses a partitioning perturbation scheme formulated by Salwen (1955). The Salwen scheme is one in which the higher order perturbation equations are only approximately solved. In the scheme we use, the higher order perturbation equations are exactly solved. We, therefore, disagree with Shirley in the first correction and in all higher corrections.

Salwen's Perturbation Scheme

The Salwen perturbation scheme is formulated for solving the problem

$$H_F|\mu\rangle = \mu|\mu\rangle \tag{XI-51}$$

where there is an almost (or exact) degeneracy in zeroth order. Let H_F have the expression

$$H_F = H_F^{(0)} + \lambda H_F^{(1)}$$

where λ is an ordering parameter. Further let $H_F^{(0)}$ have the orthonormal set of eigenfunctions, $|j\rangle$, with eigenvalues $\mu_j^{(0)}$:

$$H_F^{(0)}|j\rangle = \mu_j^{(0)}|j\rangle .$$

For simplicity, denote the two kets which are almost (or exactly) degenerate in zeroth order as $|1\rangle$ and $|2\rangle$.

Write the solution to Eq. (XI-51) as:

$$|\mu\rangle = \langle 1|\mu\rangle|1\rangle + \langle 2|\mu\rangle|2\rangle + \sum_n{}' (C_n\langle 1|\mu\rangle + D_n\langle 2|\mu\rangle)|n\rangle \tag{XI-52}$$

where the prime on the summation is used to indicate that $n = 1,2$ is to be excluded from the summation and where C_n and D_n are μ-dependent constants. By substituting Eq. (XI-52) into (XI-51) and by subsequently multiplying the result first by $\langle 1|$ and then by $\langle 2|$ we obtain the following two equations:

$$[\langle 1|H_F|1\rangle + \sum_n{}' \; C_n\langle 1|H_F|n\rangle - \mu]\langle 1|\mu\rangle + [\langle 1|H_F|2\rangle + \sum_n{}' \; D_n\langle 1|H_F|n\rangle]\langle 2|\mu\rangle = 0 \tag{XI-53}$$

$$[\langle 2|H_F|1\rangle + \sum_n{}' \; C_n\langle 2|H_F|n\rangle]\langle 1|\mu\rangle + [\langle 2|H_F|2\rangle + \sum_n{}' \; D_n\langle 2|H_F|n\rangle - \mu]\langle 2|\mu\rangle = 0 \tag{XI-54}$$

In order that there be a solution to Eqs. (XI-53) and (XI-54), the determinant of the coefficient matrix must vanish. This means that two eigenvalues of H_F are found as eigenvalues to the following 2×2 matrix:

$$\begin{pmatrix} \langle 1|H_F|1\rangle + \sum_n{}' \; C_n\langle 1|H_F|n\rangle & \langle 2|H_F|1\rangle + \sum_n{}' \; C_n\langle 2|H_F|n\rangle \\ \langle 1|H_F|2\rangle + \sum_n{}' \; D_n\langle 1|H_F|n\rangle & \langle 2|H_F|2\rangle + \sum_n{}' \; D_n\langle 2|H_F|n\rangle \end{pmatrix} \tag{XI-55}$$

That the roots of Eq. (XI-55) correspond to the perturbed eignvalues arising from states $|1\rangle$ and $|2\rangle$ may be confirmed by noting that when $\lambda \to 0$, the roots of Eq. (XI-55) are just $\mu_1^{(0)}$ and $\mu_2^{(0)}$. Of course, before finding the roots of Eq. (XI-55), we must first find the coefficients C_n and D_n. These are found by first noting the equality:

$$\langle n|H_F|\mu\rangle = \mu\langle n|\mu\rangle \qquad n \neq 1,2 . \tag{XI-56}$$

Using the expansion of $|\mu\rangle$ given by Eq. (XI-52), we have

$$\langle 1|\mu\rangle\langle n|H_F|1\rangle + \langle 2|\mu\rangle\langle n|H_F|2\rangle + \sum_j{}' (C_j\langle 1|\mu\rangle + D_j\langle 2|\mu\rangle)\langle n|H_F|j\rangle$$
$$= \mu(C_n\langle 1|\mu\rangle + D_n\langle 2|\mu\rangle) \qquad n \neq 1,2 . \tag{XI-57}$$

Eqs. (XI-57) are satisfied if we choose the coefficients C_n and D_n so that they obey:

$$\sum_j{}'' C_j\langle n|H_F|j\rangle + (\langle n|H_F|n\rangle - \mu)C_n = -\langle n|H_F|1\rangle$$
$$\sum_j{}'' D_j\langle n|H_F|j\rangle + (\langle n|H_F|n\rangle - \mu)D_n = -\langle n|H_F|2\rangle \tag{XI-58}$$

where the double prime is used to mean that $j = 1,2,n$ is to be excluded from the summation and where $n \neq 1$ or 2.

In summary then, the Salwen formulation is first to solve Eqs. (XI-58) for the coefficients C_n and D_n. These coefficients are then used to form the 2×2 matrix given by Eq. (XI-55). The roots of this matrix are two <u>exact</u> eigenvalues of (XI-51). The fly in the ointment is, of course, the fact that we must know beforehand that which we seek: we must know an exact eigenvalue, μ , before we can solve for the C_n's and D_n's since Eqs. (XI-58) depend on μ .

Solving Salwen's Equations

The formulation, so far, just changes the original problem from one in which we have a known matrix (the matrix H in the $|j\rangle$ basis) which will be difficult or impossible to diagonalize to a new problem in which we must diagonalize an unknown 2×2 matrix. Salwen, however, suggests two approaches in attempting to find the elements of the 2×2 matrix. One is an iterative scheme and the other is a perturbation scheme.

(a) The iterative scheme: The iterative scheme is simply to first select an approximate value of μ . Use this approximate value of μ in solving Eq. (XI-58) for the coefficients C_j and D_j . With these coefficients known, (XI-55) can be evaluated and then diagonalized. Select the appropriate root of (XI-55) as the new approximate value of μ with which to again carry out another iteration. Continue this cycle until a value of μ of sufficient accuracy is found. Although this is an interesting scheme of solution, we will not pursue it further here since Shirley does not use it and we are primarily interested in this report in comparing Shirley's previous work to our present work.

(b) The perturbation scheme: The specific perturbation scheme which Salwen and Shirley use is the following: Let μ which appears in Eqs. (XI-58) be given by either $\mu_1^{(0)}$ or $\mu_2^{(0)}$. Then solve

Eqs. (XI-58) perturbatively by expanding H, C_j and D_j in powers of λ. Use the perturbation approximations for C_j and D_j in forming the 2 × 2 matrix of Eq. (XI-55). The eigenvalues of the resulting matrix are taken as approximate values of μ.

Relationship of the Salwen-Shirley Perturbation Theory to Partitioning Perturbation Theory

Recall the basic equation of partitioning perturbation theory: Eq. (X-9). Assume that we know $\underset{\sim}{\chi}$ exactly where

$$\lim_{\lambda \to 0} \underset{\sim}{\chi} = (|1\rangle, |2\rangle) = \underset{\sim}{\chi}_0 . \qquad \text{(XI-59)}$$

Two exact eigenvalues of $H_F|\mu\rangle = \mu|\mu\rangle$ are recovered as roots to the following secular equation:

$$\det|\underset{\sim}{\chi}_0^\dagger (H_F - W)\underset{\sim}{\chi}| = 0 . \qquad \text{(XI-60)}$$

As the first step in explaining the Salwen-Shirley scheme write $\underset{\sim}{\chi}$ and $\underset{\approx}{E}$ as:

$$\underset{\sim}{\chi} = \underset{\sim}{\chi}_0 + \underset{\sim}{\chi}_1 ; \quad \underset{\approx}{E} = \underset{\approx}{E}_0 + \underset{\approx}{E}_1 \qquad \text{(XI-61)}$$

where $\underset{\sim}{\chi}_0$ has already been defined by Eq. (XI-59) and $\underset{\approx}{E}_0$ is, at this point, arbitrary. $\underset{\sim}{\chi}_1$ and $\underset{\approx}{E}_1$ are, therefore, correction terms which make the definitions in (XI-61) valid.

Using Eqs. (XI-61) in (X-4) we have:

$$H_F \chi_0 + H_F \chi_1 = \chi_0 E_0 + \chi_0 E_1 + \chi_1 E_0 + \chi_1 E_1 \qquad \text{(XI-62)}$$

The Certain-Hirschfelder scheme is to first take

$$E_0 = \begin{bmatrix} \mu_1^{(0)} & 0 \\ 0 & \mu_2^{(0)} \end{bmatrix}$$

and to then perturbatively solve for χ_1 and W_1. The Salwen-Shirley scheme is equivalent to first approximating Eq. (XI-62) by neglecting the term $\chi_1 E_1$. Salwen and Shirley then let

$$E_0 = \mu_j^{(0)} \, 1$$

where 1 is the 2×2 unit matrix and $\mu_j^{(0)}$ is either one of the two unperturbed almost (or exactly) degenerate eigenvalues of $H_F^{(0)}$. The resulting equation is then perturbatively solved to find χ_1 and E_1, and, approximate eigenvalues are found by then finding the roots to (XI-60). The important point to note is that the Salwen-Shirley scheme (unlike the Certain-Hirschfelder scheme) will not yield exact eigenvalues even if the perturbation theory is carried to infinite order.

Demonstrating our analysis of the Salwen-Shirley perturbation scheme in terms of the Certain-Hirschfelder theory is simple. Let the exact χ_1 be given by:

$$\underset{\sim}{\chi}_1 = \left(\sum_j{}' c_j|j>, \sum_j{}' d_j|j>\right) \qquad \text{(XI-63)}$$

where c_j and d_j are expansion coefficients and the prime means that states $|1>$ and $|2>$ are to be excluded from the summations. The eigenvalues of $H_F|\mu> = \mu|\mu>$ are found by use of Eq. (XI-60) which leads us to seek the eigenvalues of

$$\begin{pmatrix} <1|H_F|1> + \sum_j{}' c_j<1|H_F|j> & <1|H_F|2> + \sum_j{}' d_j<1|H_F|j> \\ <2|H_F|1> + \sum_j{}' c_j<2|H_F|j> & <2|H_F|2> + \sum_j{}' d_j<2|H_F|j> \end{pmatrix} \qquad \text{(XI-64)}$$

We now show that the Salwen-Shirley scheme of finding the c_j's and d_j's is equivalent to solving:

$$H_F\underset{\sim}{\chi}_0 + H_F\underset{\sim}{\chi}_1 = \underset{\sim}{\chi}_0\underset{\approx}{E}_0 + \underset{\sim}{\chi}_0\underset{\approx}{E}_1 + \underset{\sim}{\chi}_1\underset{\approx}{E}_0 \qquad \text{(XI-65)}$$

where $\underset{\sim}{\chi}_0 = (|1>,|2>)$ and $\underset{\approx}{E}_0 = \mu_j^{(0)}\,\underset{\approx}{1}$, $j = 1$ or 2 . Writing Eq. (XI-65) out explicitly we have

$$(H_F - \mu_j^{(0)})(|1> + \sum_k{}' c_k|k>) = (\underset{\approx}{E}_1)_{11}|1> + (\underset{\approx}{E}_1)_{21}|2> \qquad \text{(XI-66)}$$

$$(H_F - \mu_j^{(0)})(|2> + \sum_k{}' d_k|k>) = (\underset{\approx}{E}_1)_{12}|1> + (\underset{\approx}{E}_1)_{22}|2> \qquad \text{(XI-67)}$$

Left-multiplying both Eq. (XI-66) and Eq. (XI-67) by $<n|$ $(n \neq 1,2)$ we find that the c_j's and d_j's are determined by:

$$\sum_k{}'' c_k \langle n|H_F|k\rangle + [\langle n|H_F|n\rangle - \mu_j^{(0)}]c_n = -\langle n|H_F|1\rangle$$

(XI-68)

$$\sum_k{}'' d_k \langle n|H_F|k\rangle + [\langle n|H_F|n\rangle - \mu_j^{(0)}]d_n = -\langle n|H_F|2\rangle$$

where $n \neq 1,2$ and the double prime indicates that states $|1\rangle$, $|2\rangle$ and $|n\rangle$ are to be excluded from the summation.

Comparing Eqs. (XI-68) with Eqs. (XI-58) we see that if μ in Eqs. (XI-58) is replaced by $\mu_j^{(0)}$, c_j is the same as C_j and d_j is the same as D_j and thus our description of the Salwen-Shirley scheme in terms of the Certain-Hirschfelder partitioning is correct.

The Pegg-Series Technique: $\beta = \delta = 0$

Pegg and Series* have developed techniques to handle the problem of quantum mechanical spin systems in periodic classical fields. Pegg (1973b) applies these techniques to a study of the two-level system at its main resonance and at its subharmonic resonances. Here we discuss Pegg's application of the Pegg-Series technique to the main resonance and we defer a discussion of his treatment of the Subharmonic resonances until Chapter XII. Throughout this present section we report on Pegg's (1973b) paper although we call the technique the "Pegg-Series" technique.

To discuss the Pegg-Series technique, let us rewrite Eqs. (XI-28) in matrix notation:

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* Pegg and Series (1970) and (1973a).

$$i\dot{\underset{\approx}{A}} = \underset{\approx}{H}\,\underset{\approx}{A} \tag{XI-69}$$

where

$$\underset{\approx}{H} = \begin{pmatrix} 0 & 2\alpha\cos\tau \\ 2\alpha\cos\tau & \varepsilon \end{pmatrix}$$

The two-by-two solution matrix $\underset{\approx}{A}$ is given by

$$\underset{\approx}{A} = \begin{pmatrix} a_1(\tau) & a_2(\tau) \\ b_1(\tau) & b_2(\tau) \end{pmatrix}$$

where the solution pairs $\{a_1(\tau);b_1(\tau)\}$ and $\{a_2(\tau);b_2(\tau)\}$ form linearly independent solutions to Eq. (XI-28).

An approach to solving Eq. (XI-69) is this. Let $\underset{\approx}{S}$ be a two-by-two time-dependent matrix and let $\underset{\approx}{A}'$ be defined by

$$\underset{\approx}{A}' = \underset{\approx}{S}\,\underset{\approx}{A}$$

The equation for $\underset{\approx}{A}'$ is

$$i\dot{\underset{\approx}{A}}' = [i\dot{\underset{\approx}{S}}\,\underset{\approx}{S}^{-1} + \underset{\approx}{S}\,\underset{\approx}{H}\,\underset{\approx}{S}^{-1}]\underset{\approx}{A}' = \bar{\underset{\approx}{H}}\,\underset{\approx}{A} \tag{XI-70}$$

where $\bar{\underset{\approx}{H}}$ is defined by Eq. (XI-70) and where in deriving Eq. (XI-70) we have made use of the identity:

$$\underset{\approx}{S}\,\dot{\underset{\approx}{S}}^{-1} = -\dot{\underset{\approx}{S}}\,\underset{\approx}{S}^{-1}$$

If $\underset{\approx}{S}$ is chosen so that $\underset{\approx}{\bar{H}}$ is <u>not</u> time-dependent, we may easily and exactly solve Eq. (XI-70). For example, if $\underset{\approx}{\bar{H}}$ is a matrix of constants, we may always find a similarity transformation such that

$$\underset{\approx}{Q}^{-1}\,\underset{\approx}{\bar{H}}\,\underset{\approx}{Q} = \underset{\approx}{\Lambda} \qquad \text{(XI-71)}$$

where $\underset{\approx}{Q}$ is a nonsingular two-by-two matrix of constants and $\underset{\approx}{\Lambda}$ is a two-by-two diagonal matrix with the eigenvalues of $\underset{\approx}{\bar{H}}$ along the diagonal. If $\underset{\approx}{\bar{H}}$ is hermitian, $\underset{\approx}{Q}$ can be chosen to be a unitary matrix. The solution matrix $\underset{\approx}{A}$ is recovered by back-transforming:

$$\underset{\approx}{A} = \underset{\approx}{S}^{-1}\,\underset{\approx}{Q}\,e^{-i\underset{\approx}{\Lambda}\tau}\,\underset{\approx}{K} \qquad \text{(XI-72)}$$

where $\underset{\approx}{K}$ is an arbitrary two-by-two matrix of constants in which (in order not to get trivial solutions) we require that $\det(\underset{\approx}{K}) \neq 0$.

The basic idea behind the Pegg-Series treatment is to choose $\underset{\approx}{S}$ so that the time-dependent terms in $\underset{\approx}{\bar{H}}$ are small.* Ignoring these small terms should, therefore, give a good approximation to $\underset{\approx}{A}$.

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* Pegg (1973b) formulates the problem in terms of spin operators. Our matrix formulation is, of course, equivalent. In recent papers, Ansbacher (1973a,b) also uses a matrix formulation. Ansbacher lets $\beta = \delta = 0$ and he attempts to replace the Hamiltonian of our Eq. (I-1) by an approximate Hamiltonian, H_a , which makes the Schrödinger Equation solvable. H_a , in general, contains adjustable parameters, which Ansbacher chooses so that $(H-H_a)^2$ is minimized.

<u>Example</u>

Before describing and discussing the Pegg-Series choice of $\underset{\approx}{S}$, let us show how the Rabi Approximate solution can be derived using this formalism. To obtain the Rabi Approximate solution, let $\underset{\approx}{S}$ be defined:

$$\underset{\approx}{S} = \begin{pmatrix} e^{-i\tau/2} & 0 \\ 0 & e^{i\tau/2} \end{pmatrix} \qquad \text{(XI-73)}$$

With this choice of $\underset{\approx}{S}$, the matrix $\underset{\approx}{\bar{H}}$ is Eq. (XI-70) becomes:

$$\underset{\approx}{\bar{H}} = \begin{pmatrix} \tfrac{1}{2} & \alpha(1+e^{-2i\tau}) \\ \alpha(1+e^{2i\tau}) & \varepsilon-\tfrac{1}{2} \end{pmatrix}$$

Approximate $\underset{\approx}{\bar{H}}$ by ignoring its time-dependent terms. Doing this we are neglecting off-diagonal terms of order α. We now diagonalize the approximated $\underset{\approx}{\bar{H}}$-matrix to find

$$\underset{\approx}{\Lambda} = \tfrac{1}{2}\begin{pmatrix} \varepsilon+\sqrt{R} & 0 \\ 0 & \varepsilon-\sqrt{R} \end{pmatrix} \; ; \qquad \underset{\approx}{Q} = \begin{pmatrix} \cos\theta/2 & -\sin\theta/2 \\ \sin\theta/2 & \cos\theta/2 \end{pmatrix} \qquad \text{(XI-74)}$$

where $R = (\varepsilon-1)^2 + 4\alpha^2$, $\cos\theta = (1-\varepsilon)/\sqrt{R}$ and $\sin\theta = 2\alpha/\sqrt{R}$. Letting $\underset{\approx}{K}$ be the unit matrix, we use the Eq. (XI-74) approximations to $\underset{\approx}{\Lambda}$ and $\underset{\approx}{Q}$ in Eq. (XI-72) to recover an approximation to $\underset{\approx}{A}$. The result (aside from a normalization factor) in the same as the Rabi Approximate solutions* which we have already written in Eqs. (XI-30) and (XI-31).

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* In making the comparison we must set $\delta = 0$ in Eqs. (XI-30) and (XI-31).

The Pegg-Series Transformation

The Pegg-Series choice* of $\underset{\approx}{S}$ is written as:

$$\underset{\approx}{S} = \underset{\approx}{P}\,\underset{\approx}{V}\,\underset{\approx}{Q} \tag{XI-75}$$

where

$$\underset{\approx}{Q} = \begin{pmatrix} e^{i\tau/2} & 0 \\ 0 & e^{-i\tau/2} \end{pmatrix} ; \quad \underset{\approx}{V} = \begin{pmatrix} \cos(\theta_p/2) & \sin(\theta_p/2) \\ -\sin(\theta_p/2) & \cos(\theta_p/2) \end{pmatrix}$$

$$\underset{\approx}{P} = \begin{pmatrix} e^{iP(\tau)/2} & 0 \\ 0 & e^{-iP(\tau)/2} \end{pmatrix} \tag{XI-76}$$

θ_p is defined by

$$\cos(\theta_p) = \frac{(\varepsilon+1)}{\sqrt{R_p}} ; \quad \sin(\theta_p) = \frac{-2\alpha}{\sqrt{R_p}}$$

where $R_p = (\varepsilon+1)^2 + 4\alpha^2$. $P(\tau)$ is a function of τ and will be left unspecified at this point so that we may derive general expressions. Reading from right to left, we interpret $\underset{\approx}{S}$ in the

---

* There is a typographical error in Pegg's 1973b paper. Pegg's Equation (5) should read.

$$\hat{S}(t) = \exp\{i\,\hat{J}_z(\alpha\sin2\omega t + (p+1)\omega t\}\hat{R}^{-1}(\theta)\,\exp(-i\,\hat{J}_z\omega t)$$

Similar corrections must be made in Pegg's Equation (6). This misprint has been confirmed by Pegg in a private communication with us.

following manner. $\underset{\approx}{Q}$ represents a transformation to a reference frame which is rotating in the direction opposite to the Rabi-frame. $\underset{\approx}{V}$ diagonalizes the part of the transformed Hamiltonian which is static in this new frame. $\underset{\approx}{P}$ is chosen to make certain remaining time-dependent terms small.

With $\underset{\approx}{S}$ chosen according to Eq. (XI-75), $\underset{\approx}{\bar{H}}$ becomes:

$$
\begin{aligned}
(\underset{\approx}{\bar{H}})_{11} &= \alpha\sin(\theta_p)[1+\cos 2\tau] + \varepsilon\sin^2(\theta_p/2) - \frac{\dot{P}(\tau)}{2} - \tfrac{1}{2}\cos(\theta_p) \\
(\underset{\approx}{\bar{H}})_{12} &= \alpha e^{iP}[e^{2i\tau}\cos^2(\theta_p/2) - e^{-2i\tau}\sin^2(\theta_p/2)] \\
(\underset{\approx}{\bar{H}})_{21} &= \alpha e^{-iP}[e^{-2i\tau}\cos^2(\theta_p/2) - e^{2i\tau}\sin^2(\theta_p/2)] \\
(\underset{\approx}{\bar{H}})_{22} &= \frac{\dot{P}(\tau)}{2} + \tfrac{1}{2}\cos(\theta_p) + \varepsilon\cos^2(\theta_p/2) - \alpha\sin(\theta_p)[1+\cos 2\tau]
\end{aligned}
\qquad \text{(XI-76)}
$$

The above expressions are rigorous. In applying the Pegg-Series technique, Pegg obtains his approximation to $\underset{\approx}{\bar{H}}$ at the main resonance by

(a) Letting

$$P(\tau) = \alpha\sin(\theta_p)\sin 2\tau - 2\tau \qquad \text{(XI-77)}$$

(b) Fourier analyzing $\exp(\pm iP(\tau))$ according to:*

$$\exp[\pm iP(\tau)] = e^{\mp 2i\tau}\sum_{q=-\infty}^{\infty} J_q(\alpha\sin\theta_p)\, e^{\pm 2iq\tau} \qquad \text{(XI-78)}$$

* See Abramowitz and Stegun (1964), Eqs. 9.1.42 and 9.1.43.

where $J_q(\alpha\sin\theta_p)$ in the integer order Bessel Function of order q and argument $\alpha\sin(\theta_p)$.

(c) Retaining only the static terms which are left in $\bar{\underset{\approx}{H}}$ after steps (a) and (b).

Step (a) alone makes $(\bar{\underset{\approx}{H}})_{11}$ and $(\bar{\underset{\approx}{H}})_{22}$ static:

$$(\bar{\underset{\approx}{H}})_{11} = \tfrac{1}{2}[\varepsilon - \sqrt{R_p}] + 1$$
$$(\bar{\underset{\approx}{H}})_{22} = \tfrac{1}{2}[\varepsilon + \sqrt{R_p}] - 1 \qquad \text{(XI-79)}$$

With steps (a) and (b), the static off-diagonal terms are both equal and are both given by:

$$\alpha[\cos^2(\theta_p/2)\, J_0(\alpha\sin\theta_p) - \sin^2(\theta_p/2)\, J_2(\alpha\sin\theta_p)] \qquad \text{(XI-80)}$$

Recalling that $\varepsilon+1 \simeq 2$ at the main resonance and recalling that α is assumed to be much less than unity, we find that the largest ignored dynamic terms are of order $\mathcal{O}(\alpha^3)$.

With $\bar{\underset{\approx}{H}}$ approximated in this manner, we obtain the corresponding approximations to $\underset{\approx}{A}$ and $\underset{\approx}{Q}$. We find the Pegg-Series approximation to the solution matrix $\underset{\approx}{A}$ to be of the Floquet form. The eigenvalues of the approximated $\bar{\underset{\approx}{H}}$ matrix correspond to the Floquet characteristic exponents. Since these eignvalues were obtained by neglecting <u>off-diagonal</u> terms of order $\mathcal{O}(\alpha^3)$, they are correct through $\mathcal{O}(\alpha^5)$. The corresponding eigenvectors (correct through $\mathcal{O}(\alpha^2)$) are involved in the expressions for the "ϕ-parts" of the Floquet Normal Modes.

A disadvantage to the Pegg-Series technique is that the transformation are <u>ad hoc</u> and there is no prescription for obtaining solutions of arbitrary accuracy. Furthermore, the Pegg-Series technique is not applicable when β does not vanish.

<u>The relationship of the Pegg-Series technique to partitioning perturbation theory.</u>

Relating the matrix formulation outlined above to the partitioning theory outlined in Chapter X is straightforward. Let $\underset{\approx}{A}$ be the Floquet solutions:

$$\underset{\approx}{A} = \underset{\approx}{\Phi}_F \, e^{-i\underset{\approx}{\mu}_F \tau} \tag{XI-81}$$

where

$$\underset{\approx}{\Phi}_F = \begin{pmatrix} \phi_{a1} & \phi_{a2} \\ \phi_{b1} & \phi_{b2} \end{pmatrix} ; \qquad \underset{\approx}{\mu}_F = \begin{pmatrix} \mu_1 & 0 \\ 0 & \mu_2 \end{pmatrix}$$

The μ_j's $(j = 1,2)$ are the characteristic exponents and the ϕ_{ij}'s are the periodic parts of the Floquet solutions. Using Eq. (XI-81) in Eq. (XI-69) we find after first left multiplying the result by $\exp[i\underset{\approx}{\mu}_F\tau]$ and then right multiplying the result by $\underset{\approx}{\Phi}_F^{-1}$ that

$$\underset{\approx}{\mu}_F = [i\dot{\underset{\approx}{\Phi}}_F^{-1}\underset{\approx}{\Phi}_F + \underset{\approx}{\Phi}_F^{-1}\underset{\approx}{H}\,\underset{\approx}{\Phi}_F] \tag{XI-82}$$

By comparing Eq. (XI-82) with Eq. (XI-70) we see that a transformation matrix which makes $\bar{\underset{\approx}{H}}$ in Eq. (XI-70) both static and diagonal is the choice:

$$\underset{\approx}{S} = \underset{\approx}{\Phi}_F^{-1}$$

From Eq. (III-19), $\det(\underset{\approx}{\Phi}_F)$ is nonvanishing for all values of τ and thus $\underset{\approx}{\Phi}_F^{-1}$ exists for all τ . Note that if we make the choice

$$\underset{\approx}{S} = \underset{\approx}{c}\ \Phi_F^{-1} \qquad \text{(XI-83)}$$

where $\underset{\approx}{c}$ is a nonsingular two-by-two square matrix of constants, the matrix $\bar{\underset{\approx}{H}}$ in Eq. (XI-70) becomes

$$\bar{\underset{\approx}{H}} = \underset{\approx}{c}\ \underset{\approx}{\mu}_F\ \underset{\approx}{c}^{-1}$$

which is clearly a (in general, nondiagonal) constant matrix. The transformation matrix given by (XI-83) contains $\underset{\approx}{c}$. The matrix $\underset{\approx}{c}$ merely linearly combines (or scrambles) the elements of $\underset{\approx}{\Phi}_F^{-1}$. Since the partitioning theory is equivalent to finding linear combinations of the ϕ-parts of the Floquet solutions, the partitioning theory is a way of systematically finding a matrix $\underset{\approx}{S}$ which makes $\bar{\underset{\approx}{H}}$ static. Pegg's method differs from the partitioning theory in that his transformations are ad hoc and in that he gives no method of systematically finding $\underset{\approx}{S}$ to arbitrary accuracy.

The Silverman and Pipkin Technique: $\beta = 0$; $\delta \neq 0$.

Silverman and Pipkin (1972) have studied the two-level system at its main resonance allowing for decay. They use the matrix formulated which we have just outlined in describing the Pegg-Series technique. Since they consider decay, let ε in Eq. (XI-69) be replaced by $(\varepsilon - i\delta)$.

Their choice of $\underset{\approx}{S}$ is the same as Pegg's choice (see Eq. (XI-75)) except:

(a) $P(\tau) = 2\tau$

(b) In the matrix $\underset{\approx}{V}$ replace θ_p by θ_s where

$$\cos\theta_s = \frac{\varepsilon - i\delta + 1}{\sqrt{R_s}} \, ; \qquad \sin\theta_s = \frac{-2\alpha}{\sqrt{R_s}}$$

$$R_s = (\varepsilon - i\delta + 1)^2 + 4\alpha^2$$

Note that because of the inclusion of nonvanishing δ , the $\underset{\approx}{S}$-matrix is no longer hermitian. Silverman and Pipkin use this transformation to obtain $\underset{\approx}{\bar{H}}$. $\underset{\approx}{\bar{H}}$ is then approximated by retaining <u>only</u> static terms. This procedure gives an approximated $\underset{\approx}{\bar{H}}$-matrix of the form:*

---

* Silverman and Pipkin's Eq. (35) is wrong. The off-diagonal elements in their $\underset{\approx}{M}_R$ matrix should be divided by $(1 + \kappa_A^2)$. The algebraic results following from (35) are therefore erroneous. Professor Pipkin has confirmed these observations in a private communication with us.

$$(\underset{\approx}{\bar{H}})_{11} = \tfrac{1}{2}[\varepsilon - i\delta - \sqrt{R_s}] - 1 \; ; \quad (\underset{\approx}{\bar{H}}_{22}) = \tfrac{1}{2}[\varepsilon - i\delta + \sqrt{R_s}] + 1$$
$$(\underset{\approx}{\bar{H}})_{12} = (\underset{\approx}{\bar{H}})_{21} = -\alpha\sin^2(\theta_s/2) \qquad \text{(XI-84)}$$

In obtaining this approximation to $\underset{\approx}{\bar{H}}$, they neglect diagonal terms of magnitude $\mathcal{O}(\alpha^2)$ and of periodicity π . They neglect off-diagonal terms of magnitude $\mathcal{O}(\alpha)$ and of periodicity $(\pi/2)$.

In back-transforming to obtain $\underset{\approx}{A}$, their procedure yields Floquet solutions correct through $\mathcal{O}(\alpha)$ in the characteristic exponents and correct through $\mathcal{O}(\alpha^0)$ in the periodic parts of the Floquet solutions.

Like the Pegg-Series technique, the Silverman-Pipkin technique lacks ease of extension to obtain results of arbitrary accuracy.

<u>Winter's Technique: $\beta \neq 0$, $\delta = 0$.</u>

Winter (1959) has studied the main as well as subharmonic resonances of two-level system. He has considered the case of nonvanishing β . He does not, however, allow for nonvanishing values of δ .

Although he does not explicitly mention the Floquet theory, he derives solutions of the Floquet form. He uses a perturbation theory which, although outwardly different in its formal development, is equivalent to the Certain-Hirschfelder theory. Since he is primarily concerned with the subharmonic resonances, we defer a more complete discussion of Winter's work until the end of Chapter XII.

<u>The Case of $\beta \neq 0$ and $\delta \neq 0$.</u>

We have found no previous work which considers both nonvanishing β <u>and</u> nonvanishing δ . In Part I of this section, however, we have given a method of solving for this general case to any desired degree of accuracy.

XII. PARTITIONING PERTURBATION THEORY APPLIED TO THE SUB-HARMONIC RESONANCES

Introduction

This chapter is split into two parts. In Part I we show that when $\varepsilon \approx n_r$ (where n_r is some integer greater than unity), the sub-harmonic resonances are treated either by the Technique T7, which we shall introduce here, or by Technique T1 which has already been discussed in Chapter VIII. Which technique to use is determined by the values of n_r, β and N, where, throughout this chapter, we define N to be the order of field strength through which the "ϕ-parts" of the Floquet solutions are correct. Figure (XII-A) is a flow chart which summarizes when to use Technique T7 and when to use Technique T1 depending upon the values of N, n_r and β.

In the second part of this chapter we compare our treatment of the sub-harmonic resonances to the work of Shirley (1963,1965) and Winter (1959). We also discuss Pegg's (1973b) work in which Pegg uses the Pegg-Series technique to treat the sub-harmonic resonances.

Part I: Solutions for a Sub-Harmonic Resonance

Technique T7 is just the partitioning perturbation theory in which we define

$$\underset{\sim}{\chi}^{(0)} = (|A,0\rangle, |B,-n_r\rangle) \qquad \text{(XII-1)}$$

Technique T7 therefore consists of the following steps:*

Steps to follow in using Technique T7.

Step (1). Let $\underset{\sim}{\chi}^{(0)} = (|A,0>, |B,-n_r>)$ because, by hypothesis, the states $|A,j>$ and $|B,j-n_r>$ are almost degenerate with respect to $H_F^{(0)}$. Since the final time-dependent results are invariant to the choice of j , for the sake of simplicity choose $j = 0$.

Step (2). Solve Eq. (X-9) by using perturbation theory after H_F , $\underset{\sim}{\chi}$ and $\underset{\approx}{E}$ have been expanded in powers of the field strength. The first three perturbation equations have already been explicitly written out in Eqs. (X-17), (X-18) and (X-19). Furthermore, it is convenient to use intermediate normalization in solving the perturbation equations:

$$<k,j|\chi_\ell^{(n)}> \quad = \quad 0 \qquad \text{(XII-2)}$$

where $n > 0$; ℓ = a or b ; $(k,j) = (A,0)$ or $(B,-n_r)$.

Step (3). Form the secular equation, Eq. (X-23). The elements of this secular equation are defined by Eq. (X-13a).

Step (4). Diagonalize Eq. (X-23). The eigenvalues correspond to the Floquet characteristic exponents and they are correct through (2N+1)-th order in the field strength. By using Eqs. (X-24), (V-7)

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* The partitioning perturbation theory is fully discussed in Chapter X. An example of its application to the main resonance has been given in Chapter XI.

and (V-8), the eigenvectors associated with each root are used to find the Fourier coefficients correct through N-th order in the field strength.

Techniques T1 and T7 applied to the sub-harmonic resonances.

Two different techniques T1 and T7 are used in treating the sub-harmonic resonances. This is so because when partitioning perturbation is applied to the sub-harmonic resonances, we are led to a partitioning secular equation (Eq. (X-23)) in which off-diagonal elements vanish for certain values of N, n_r and β. When the off-diagonal elements of Eq. (X-23) vanish, the partitioning solutions are equivalent to the non-degenerate Rayleigh-Schrödinger results and therefore T1 and T7 differ only in normalization.

Figure (XII-A) diagrammatically shows when to use T1 and when to use T7 depending on the values of β, N and n_r. The spirit of Figure (XII-A) is this. Suppose that N, n_r and β are such that the application of partitioning theory leads to vanishing off-diagonal elements. We have therefore used a new technique (T7) to obtain results equivalent to results already obtained by an old technique (T1). So why not save time and energy and figure out when this is going to occur beforehand? Figure (XII-A) does just this.

We arrive at Figure (XII-A) by detailed consideration of the $\underset{\sim}{\chi}_a(N)$'s and $\underset{\sim}{\chi}_b(N)$'s where $N = 0,1,2,\ldots$etc. Consider first $N = 0$.

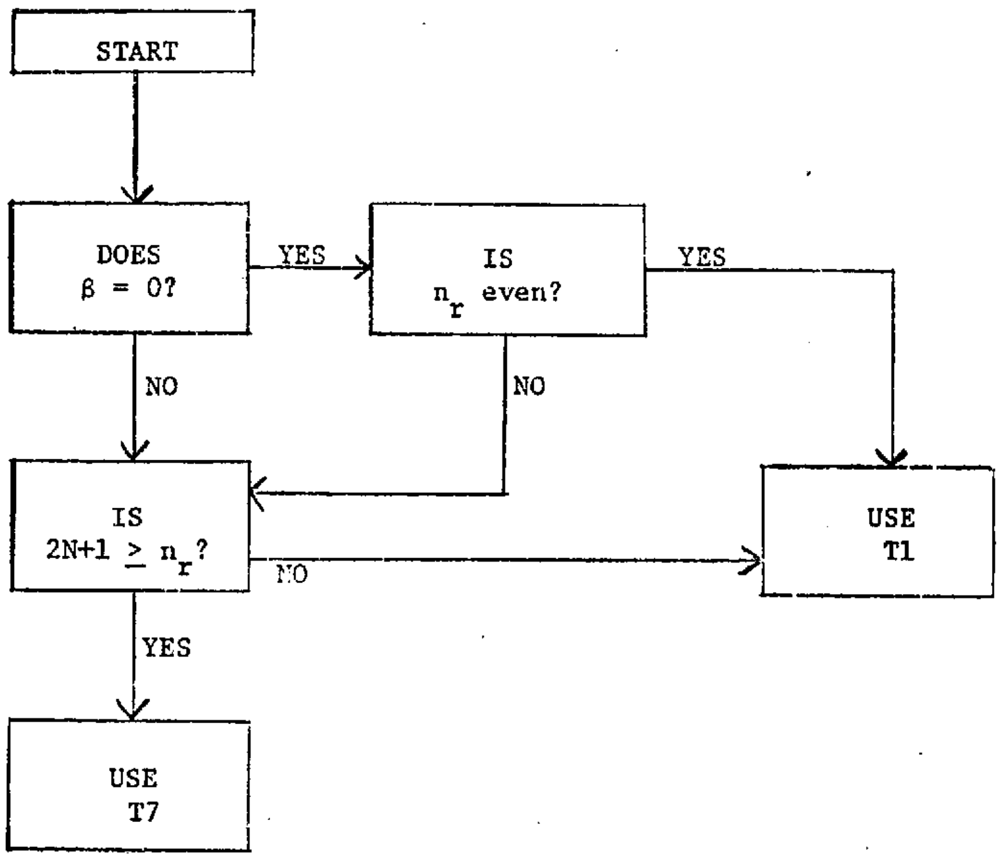

FIGURE (XII-A). Best technique to use to obtain $a(\tau)$ and $b(\tau)$ correct through N-th order in the field strength when $\varepsilon \simeq n_r$ (n_r any integer greater than zero) and α, β and δ are all much less than unity.

N = 0

If $N = 0$, then $\chi_a^{(0)} = \chi_a(0) = |A,0>$ and $\chi_b^{(0)} = \chi_b(0) = |B,-n_r>$. $H_F|\chi_a(0)>$ therefore has components in

$$[|A,0>,|B,\pm 1>] \tag{XII-3}$$

By this we mean that $<k,j|H_F|\chi_a(0)>$ vanishes unless $(k,j) = (A,0)$ or $(B,\pm 1)$.

$H_F|\chi_b(0)>$ has components in

$$[|B,-n_r>,|A,-n_r\pm 1>,\beta|B,-n_r\pm 1>] \tag{XII-4}$$

By this we mean that $<k,j|H_F|\chi_b(0)>$ vanishes unless $(k,j) = (B,-n_r),(A,-n_r\pm 1)$ or $(B,-n_r\pm 1)$. Furthermore, if any of the kets which appear in the brackets are multiplied by β, then there are no components of those kets in $H_F|\chi_b(0)>$ when the parameter β vanishes. Thus, if $\beta = 0$, $H_F|\chi_b(0)>$ has no components in $|B,-n_r\pm 1>$. This notation and phaseology is used throughout the present discussion.

From the definition of $\underset{\sim}{\chi}(0)$ and from the expressions (XII-3) and (XII-4), we see that when $N = 0$, Eq. (X-23) has off-diagonal elements only if $n_r = 1$. This is true regardless of the value of β.

N = 1

If $N = 1$, from the first order partitioning perturbation equations (Eq. (X-18)) and from the normalization

$$\langle k,j|\chi_a^{(n)}\rangle = \langle k,j|\chi_b^{(n)}\rangle = 0$$

$$n \geq 1 \; ; \quad (k,j) = (A,0) \text{ or } (B,-n_r)$$

it is clear than $\chi_a(1)$ has components in:

$$[|A,0\rangle, |B,\pm 1\rangle] \tag{XII-5}$$

$\chi_b(1)$ has components in:

$$[|B,-n_r\rangle, |A,-n_r\pm 1\rangle, \beta|B,-n_r\pm 1\rangle] \tag{XII-6}$$

$H_F\chi_a(1)$ has components in:

$$[|A,0\rangle, |B,\pm 1\rangle, |A,\pm 2\rangle, \beta|B,0\rangle, \beta|B,\pm 2\rangle] \tag{XII-7}$$

and $H_F\chi_b(1)$ has components in:

$$[|B,-n_r\rangle, |A,-n_r\pm 1\rangle, |B,-n_r\rangle, |B,-n_r\pm 2\rangle, \beta|B,-n_r\pm 1\rangle, \beta|A,-n_r\pm 2\rangle, \beta|A,-n_r\rangle] \tag{XII-8}$$

Knowing the components of $\chi_j(1)$ and $H_F\chi_j(1)$ $(j = a,b)$, it is easy to see that if $N = 1$ in Eqs. (X-23), Eq. (X-23) will have non-vanishing off-diagonal elements

(a) if $\beta \neq 0$, only when $n_r \leq 3$.

(b) if $\beta = 0$, only when $n_r = 1$ or 3 .

N = 2

Forming the partitioning secular equation with $N = 2$, from considerations exactly similar to those in the above discussions, we find non-vanishing off-diagonal elements

(a) If $\beta \neq 0$, only when $n_r \leq 5$

(b) If $\beta = 0$, only when $n_r = 1,3$ or 5 .

N < 2

From consideration of the cases of $N < 2$ as well as the cases $N = 0,1,2$, we find the following behavior:

The off-diagonal elements of Eq. (X-23) are non-vanishing only under the following two sets of conditions:

(a) if $\beta \neq 0$, only when $n_r \leq (2N+1)$

(b) if $\beta = 0$, only when $n_r \leq (2N+1)$ and n_r is odd.

The consequences of these two sets of conditions are summarized by Figure (XII-A).

The Technique T1 convergence requirements if $\beta = 0$.

The Technique T1 convergence requirements were given in Eqs. (VIII-13). It was stipulated that

$$|K_{min} - \varepsilon| \gg \alpha,\beta$$

where K_{min} is the integer (including zero) which makes $|K_{min}-\varepsilon|$ as small as possible. When $\beta = 0$, however, T7 is equivalent to

T1. This means that for $\beta = 0$, denominators of the form, $|K'_{min} - \varepsilon|$, where K'_{min} is an even (non-zero) integer, never occur.

<u>If $\beta = 0$</u> , the non-degenerate Rayleigh-Schrödinger perturbation series (the T1 solutions) will quickly converge if

$\alpha << 1$; $|K'_{min}-\varepsilon| >> \alpha$; δ arbitrary. K'_{min} is the <u>odd</u> integer (or zero) which makes $|K'_{min}-\varepsilon|$ as small as possible.

(XII-9)

As Winter (1959) has shown, there is a physical manifestation of the fact that when $\beta = 0$ and n_r is even the T1 solutions are the appropriate solutions. If $\beta = 0$, a two-level system shows resonance absorption peaks only at values of ε equal (or almost equal) to an odd integer. If, on the other hand, $\beta \neq 0$, a two-level system shows resonance absorption peaks at <u>all</u> integer values of ε . Margerie and Brossel (1955) were the first investigators to experimentally observe the sub-harmonic resonances. They observed radio frequency transitions in sodium vapor corresponding to $\varepsilon = 1,2,3$ and 4 .

<u>Part II: Other Treatments of the Two-Level System's Sub-Harmonic Resonances.</u>

<u>Shirley's Approach: $\beta = \delta = 0$</u>

The approach we have just used to treat the sub-harmonic resonances is basically Shirley's (1963,1965) technique extended to account for non-vanishing values of β and δ . The only difference between our approach and Shirley's approach is that we solve the perturbation equations exactly.

We have already discussed Shirley's perturbation theory in Chapter XI. All the results, discussion, conclusions, etc. apply here.

The Pegg-Series Technique: $\beta = \delta = 0$

In his (1973b) paper, Pegg uses the Pegg-Series technique to obtain solutions for the two-level system's sub-harmonic resonances. Since we have already discussed the Pegg-Series technique fully in Chapter XI, we assume the reader's familiarity with the ideas and notation contained in that discussion.

In considering $\varepsilon \approx n_r$ (n_r here can be any integer greater than zero), Pegg (1973b) suggests that the transformation $\underset{\sim}{S}$ be defined just as we defined it in Eq. (XI-75) <u>except</u> that, for the general n_r , $P(\tau)$ be defined by

$$P(\tau) = \alpha\sin(\theta_p)\sin 2\tau - 2n_r\tau \qquad \text{(XII-10)}$$

where θ_p has already been defined in the discussion following Eq. (XI-75). Clearly, for $n_r = 1$, Eq. (XII-10) reduces to Eq. (XI-77).

Just as we did in Chapter XI, we form the matrix $\bar{\underset{\approx}{H}}$ ($\bar{\underset{\approx}{H}}$ has been defined by Eq. (XI-70)). After Fourier analyzing $\exp[\pm iP(\tau)]$ according to

$$\exp[\pm iP(\tau)] = e^{\mp 2in_r\tau} \sum_{q=-\infty}^{\infty} J_q(\alpha\sin\theta_p)\, e^{\pm 2iq\tau} \qquad \text{(XII-11)}$$

where the functions $J_q(\alpha\sin\theta_p)$ have already been defined by Eq. (XI-78), we retain only the <u>static</u> terms of $\bar{\underset{\approx}{H}}$. No dynamic terms must be ignored in the diagonal part of $\bar{\underset{\approx}{H}}$ and the diagonal part of $\bar{\underset{\approx}{H}}$ is given by

$$\begin{aligned} (\bar{\underset{\approx}{H}})_{11} &= \tfrac{1}{2}[\varepsilon - \sqrt{R_p}] + n_r \\ (\bar{\underset{\approx}{H}})_{22} &= \tfrac{1}{2}[\varepsilon + \sqrt{R_p}] - n_r \end{aligned} \qquad \text{(XII-12)}$$

For the case of $n_r = 1$, Eqs. (XII-12) reduce to Eqs. (XI-79).

The static off-diagonal terms of $\bar{\underset{\approx}{H}}$ are both equal and are given by:

$$\alpha[\cos^2(\theta_p/2)J_{n_r-1}(\alpha\sin\theta_p) - \sin^2(\theta_p/2)J_{n_r+1}(\alpha\sin\theta_p)] \qquad \text{(XII-13)}$$

For $n_r = 1$, Eq. (XII-13) reduces to Eq. (XI-80). Just as before, the Pegg-Series prescription is to approximate $\bar{\underset{\approx}{H}}$ by its static part. This approximate $\bar{\underset{\approx}{H}}$ leads to approximate expressions for the Floquet Normal Mode solutions.

When $n_r \neq 1$, however, we <u>always</u> neglect a dynamic term proportional to

$$\alpha\cos^2(\theta_p/2)J_0(\alpha\sin\theta_p) \qquad \text{(XII-14)}$$

This term is of order $O(\alpha)$ and the Pegg-Series prescription for the sub-harmonic resonances leads to Floquet solutions correct through $O(\alpha)$ in the characteristic exponents and correct only through zeroth order in the "ϕ-parts" of the Floquet Normal Modes.

Because of its low formal accuracy and because of its *ad hoc* nature, we do not recommend using the Pegg-Series technique in treating the sub-harmonic resonances.

Winter's Treatment: $\beta \neq 0$ and $\delta = 0$

Winter (1959) considers the sub-harmonic resonances with β non-vanishing and δ vanishing. Although his end results are just our results, his formulation of the steps leading to these equivalent results is quite different from our formulation. The differences occur both in the transformation of the dynamic problem into a static problem and in the solution of the static problem in the regime of near (or exact) degeneracies.

Transformation to a Static Problem

Winter considers equations equivalent to Eqs. (II-4) and (II-5) under the stipulation that $\delta = 0$:

$$\begin{aligned} \dot{a} &= -2i\alpha\cos\tau b \\ \dot{b} &= -i\varepsilon b - 2i\beta\cos\tau b - 2i\alpha\cos\tau a \end{aligned} \qquad \text{(XII-15)}$$

Rather than directly using Floquet's Theorem, he makes the ansatz that $a(\tau)$ and $b(\tau)$ may be written as:

$$a(\tau) = \sum_{n=-\infty}^{\infty} a_n(\tau)\, e^{in\tau} \qquad \text{(XII-16)}$$

$$b(\tau) = \sum_{n=-\infty}^{\infty} b_n(\tau)\, e^{in\tau} \qquad \text{(XII-17)}$$

where the $a_n(\tau)$'s and $b_n(\tau)$'s are <u>functions</u> <u>not</u> <u>constants</u>. First letting

$$\cos\tau = \tfrac{1}{2}(e^{i\tau} + e^{-i\tau})$$

and then substituting (XII-16) and (XII-17) into Eqs. (XII-15), Winter matches terms multiplying each and every $e^{ij\tau}$ to obtain the following equations for the functions $a_n(\tau)$ and $b_n(\tau)$:

$$\dot{a}_n(\tau) = -ina_n(\tau) - i\alpha[b_{n-1}(\tau) + b_{n+1}(\tau)]$$

$$\text{(XII-18)}$$

$$\dot{b}_n(\tau) = -i(\varepsilon+n)b_n(\tau) - i\beta[b_{n-1}(\tau) + b_{n+1}(\tau)] - i\alpha[a_{n-1}(\tau) + a_{n+1}(\tau)]$$

where n ranges from $-\infty$ to ∞ .

Notice that Eqs. (XII-18) are an infinite set of linear, homogeneous coupled differential equations with constant coefficients. They have a solution of the form

$$a_n(\tau) = e^{-i\mu\tau} A_n$$

$$\text{(XII-19)}$$

$$b_n(\tau) = e^{-i\mu\tau} B_n$$

where μ , the A_n's and B_n's are constants. Using Eqs. (XII-19) in (XII-18) we arrive at exactly the same matrix eigenvalue-eigenvector equation which we have already written as Eq. (III-35). Thus, the μ in Eq. (XII-19) corresponds to a Floquet characteristic exponent and the A_n's and B_n's in Eq. (XII-19) are exactly the Fourier Expansion coefficients of Eqs. (III-34). Therefore, although Winter never invokes Floquet's Theorem or Fourier's Theorem, he implicitly uses them to recast the time-dependent problem into the static eigenvalue-eigenvector problem which we have already given by Eq. (III-35).

The Winter-Heitler Perturbation Theory

Winter recognizes that resonances occur when $\varepsilon \approx n_r$ and that resonances correspond to near (or exact) degeneracies in the $\underset{\approx}{M}$ matrix (see Eq. (III-36) for $\underset{\approx}{M}$'s definition). To handle the problem of near degeneracies, Winter extends a formalism due to Heitler.* At first glance, the Winter-Heitler Perturbation Theory appears different than the Certain-Hirschfelder partitioning perturbation theory. We show, however, that the two are equivalent if "Certain-full-normalization" is used in the partitioning theory.

In explaining the Winter-Heitler theory, it is convenient to replace the (B,j)-th row of $\underset{\approx}{M}$ by its $(B,j-n_r)$-th row $(j = -\infty,\ldots,\infty)$ to generate a new matrix $\underset{\approx}{M}'$. The rows and columns of $\underset{\approx}{M}'$ are still ordered according to

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* Heitler (1960), Chapter 4, Section 14.

$$\ldots A_1, B_1, A_0, B_0, A_{-1}, B_{-1}, \ldots \qquad \text{(XII-20)}$$

and, by definition, we therefore have,

$$(\underset{\approx}{M}')_{A,j;k,\ell} = (\underset{\approx}{M})_{A,j;k,\ell}$$

$$(\underset{\approx}{M}')_{B,j;k,\ell} = (\underset{\approx}{M})_{B,j-n_r;k,\ell}$$

where $k = A$ or B and $\ell = -\infty,\ldots,\infty$. $\underset{\approx}{M}'$ has been defined so that the almost degenerate pairs

$$j \quad \text{and} \quad j + \varepsilon - n_r$$

occur adjacent to each other along the diagonal of $\underset{\approx}{M}'$. Further define the column vector $\underset{\sim}{C}'$ in terms of the vector $\underset{\sim}{C}$ of Eq. (III-35). The elements of $\underset{\sim}{C}'$ are ordered according to (XII-20) and therefore:

$$\begin{aligned} (\underset{\sim}{C}')_{B,j} &= (\underset{\sim}{C})_{B,j-n_r} \\ (\underset{\sim}{C}')_{A,j} &= (\underset{\sim}{C})_{A,j} \end{aligned} \qquad \text{(XII-21)}$$

where $j = -\infty,\ldots,\infty$. It is evident that the problem $(\underset{\approx}{M}-\mu\underset{\approx}{I})\underset{\sim}{C} = 0$ is exactly equivalent to the problem

$$(\underset{\approx}{M}'-\mu\underset{\approx}{I})\underset{\approx}{C}' = 0 \qquad \text{(XII-22)}$$

It is this latter problem to which the Winter-Heitler perturbation theory is applied.

$\underset{\approx}{M}'$ still has almost (or exact) degeneracies along its diagonal:

$$(\underset{\approx}{M}')_{A,j;A,j} \approx (\underset{\approx}{M}')_{B,j;B,j}$$

To overcome the difficulties which these near (or exact) degeneracies cause in the perturbation solution of Eq. (XII-22), a unitary transformation, $\underset{\approx}{S}$, is sought which has the property

$$\underset{\approx}{S}^{\dagger}\,\underset{\approx}{M}'\,\underset{\approx}{S} = \underset{\approx}{K} \; ; \quad \underset{\approx}{S}^{\dagger}\,\underset{\approx}{S} = \underset{\approx}{I} \qquad \text{(XII-23)}$$

where $\underset{\approx}{I}$ is the infinite unit matrix and $\underset{\approx}{K}$ is an infinite square matrix. The rows and columns of $\underset{\approx}{K}$ are ordered according to (XII-20) and $\underset{\approx}{K}$ is defined so that all its elements vanish except its diagonal elements and the elements:

$$(\underset{\approx}{K})_{A,j;B,j} \; ; \quad (\underset{\approx}{K})_{B,j;A,j}$$

With $\underset{\approx}{S}$ and $\underset{\approx}{K}$ defined in this manner, Eq. (XII-22) becomes:

$$(\underset{\approx}{S}^{\dagger}\,\underset{\approx}{M}'\,\underset{\approx}{S} - \mu\underset{\approx}{I})(\underset{\approx}{S}^{\dagger}\,\underset{\sim}{C}') = (\underset{\approx}{K} - \mu\underset{\approx}{I})(\underset{\approx}{S}^{\dagger}\,\underset{\sim}{C}') = 0 \quad \text{(XII-24)}$$

Since $\underset{\approx}{K}$ is block diagonal with 2×2 matrices along its diagonal, solving Eq. (XII-24) is a simple task. The difficult task is to find

$\underset{\approx}{S}$ and $\underset{\approx}{K}$. Winter suggests that they be found by a field-strength perturbation solution to

$$\underset{\approx}{M}' \underset{\approx}{S} = \underset{\approx}{S} \underset{\approx}{K} \qquad \text{(XII-25)}$$

We show that the Winter-Heitler procedure is equivalent to the Certain-Hirschfelder treatment by noting that the $\underset{\approx}{S}$ matrix is merely a matrix containing "scrambled" eigenvectors of $\underset{\approx}{M}'$. Since the Certain-Hirschfelder treatment also seeks scrambled eigenvectors of $\underset{\approx}{M}'$, the two treatments are equivalent if Certain-full-normalization* is required in the Certain-Hirschfelder treatment.

We demonstrate this assertion by first denoting the exact eigenvalues and eigenvectors of $\underset{\approx}{M}'$ by:

$$\underset{\approx}{M}' \underset{\sim}{C}'_{k,\ell} = \mu_{k,\ell} \underset{\sim}{C}'_{k,\ell} \qquad \text{(XII-26)}$$

where $k = A$ or B and $\ell = -\infty, \ldots, \infty$. The complete solution to Eq. (XII-22) is written as

$$\underset{\approx}{M}' \underset{\approx}{C}' = \underset{\approx}{C}' \underset{\approx}{\mu} \qquad \text{(XII-27)}$$

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* By this we mean that when, H_F is Hermitian (i.e., $\delta = 0$), we choose $\underset{\approx}{c}$ of our Eq. (X-7) to be unitary. See Certain and Hirschfelder's (1970a) paper for more details.

where $\underset{\approx}{C}'$ and $\underset{\approx}{\mu}$ are infinite square matrices, and, the rows and columns of both are ordered according to (XII-20). The (k,ℓ)-th column of $\underset{\approx}{C}'$ contains the solution vector $\underset{\sim}{C}'_{k,\ell}$ and $\underset{\approx}{\mu}$ is diagonal and

$$(\underset{\approx}{\mu})_{k,\ell;k,\ell} = \mu_{k,\ell}$$

where $k = A$ or B and $\ell = -\infty,\ldots,\infty$. Since $\underset{\approx}{C}'$ contains the eigenvectors or a real, symmetric matrix,

$$(\underset{\approx}{C}')^{\dagger}\,\underset{\approx}{C}' = \underset{\approx}{I}$$

where $\underset{\approx}{I}$ is the infinite unit matrix.

Define an infinite set of arbitrary 2×2 unitary matrices, $\underset{\approx}{\nu}(j)$ where $j = -\infty,\ldots,\infty$. Further define an infinite square matrix $\underset{\approx}{V}$ the rows and columns of which are ordered according to (XII-20). $\underset{\approx}{V}$ is block diagonal having the matrices $\underset{\approx}{\nu}(j)$ along its diagonal. Therefore, all elements of $\underset{\approx}{V}$ are zero except:

$$\begin{aligned}
(\underset{\approx}{V})_{A,j;A,j} &= (\underset{\approx}{\nu}(j))_{11} \\
(\underset{\approx}{V})_{B,j;B,j} &= (\underset{\approx}{\nu}(j))_{22} \\
(\underset{\approx}{V})_{B,j;A,j} &= (\underset{\approx}{\nu}(j))_{21} \\
(\underset{\approx}{V})_{A,j;B,j} &= (\underset{\approx}{\nu}(j))_{12}
\end{aligned} \qquad \text{(XII-28)}$$

We now assert that $\underset{\approx}{S}$ is simply given by

$$\underset{\approx}{S} = \underset{\approx}{C}' \, \underset{\approx}{V} \, . \qquad \text{(XII-29)}$$

$\underset{\approx}{S}$ is unitary and it is composed of "scrambled" (or linearly combined) eigenvectors of $\underset{\approx}{M}'$. With $\underset{\approx}{S}$ defined by Eq. (XII-29), we have:

$$\underset{\approx}{S}^{\dagger} \, \underset{\approx}{M}' \, \underset{\approx}{S} = \underset{\approx}{V}^{\dagger} (\underset{\approx}{C}')^{\dagger} \, \underset{\approx}{M}' \, \underset{\approx}{C}' \, \underset{\approx}{V} = \underset{\approx}{V}^{\dagger} \, \underset{\approx}{\mu} \, \underset{\approx}{V} \qquad \text{(XII-30)}$$

From the definitions of $\underset{\approx}{\mu}$ and $\underset{\approx}{V}$ it is clear that $\underset{\approx}{V}^{\dagger} \, \underset{\approx}{\mu} \, \underset{\approx}{V}$ may be identified with $\underset{\approx}{K}$. Therefore, the Winter-Heitler and Certain-Hirschfelder treatments are equivalent as long as Certain-full-normalization is used in the latter.

XIII. TECHNIQUE T8: THE $(1/\varepsilon)$-EXPANSION OF THE QUOTIENT EQUATIONS APPLIED TO $\varepsilon >> 1$ AND (2α), (2β) AND δ ALL MUCH LESS THAN ε

Introduction

In this section we present perturbation solutions of Eqs. (II-4) and (II-5) which are useful for the following ranges of the parameters:

$\varepsilon >> 1$ and (2α), (2β) and δ are all much less than ε .

In Technique T8 we do not directly deal with Eqs. (II-4) and (II-5). Rather we solve the equation for $b(\tau)/a(\tau)$ to find one of the Floquet Modes as a power series in inverse powers of ε . We then solve the equation for $a(\tau)/b(\tau)$ to find the other Floquet Mode as a power series in inverse powers of ε . We believe that this is a new way of obtaining solutions for the two-state time-dependent problem.

There are two solutions for $b(\tau)/a(\tau)$ as a series in powers of $(1/\varepsilon)$. One of these series has terms in $(1/\varepsilon)^n$ where $n = 1,2,3,\ldots$ and corresponds to one of the Floquet Modes. The other power series has terms with $n = -1,0,1,\ldots$ and (although it corresponds to the other Floquet Normal Mode) it is not useful for us since many of the individual terms become infinite for particular values of τ . Similarly, there are two series in powers of $(1/\varepsilon)$ for $a(\tau)/b(\tau)$. The series with $n = 1,2,3,\ldots$ corresponds to the Second Floquet Mode. Again, the solution with $n = -1,0,1,\ldots$ is not useful.

Knowing an asymptotically convergent series for <u>one</u> of the Floquet solutions to $b(\tau)/a(\tau)$ <u>and</u> an asymptotically convergent series for the <u>inverse</u> of the other Floquet solution to $b(\tau)/a(\tau)$, we construct approximations to the two linearly independent Floquet solutions of Eqs. (II-4) and (II-5). We may linearly combine these latter solutions to obtain a $(1/\varepsilon)$ expansion of a solution to Eqs. (II-4) and (II-5) obeying arbitrary initial conditions.

Although the equations for $b(\tau)/a(\tau)$ and $a(\tau)/b(\tau)$ appear to be singular perturbations in the parameter $(1/\varepsilon)$, when $\delta = 0$ their solutions do not approach an "outer" solution as τ becomes large. This anomalous behavior and also the convergence of the series is discussed at the end of this chapter.

<u>Statement of Quotient Equations</u>

Let

$$a(\tau) = e^{\theta_1(\tau)} \; ; \quad b(\tau) = \Phi_1(\tau)e^{\theta_1(\tau)} \qquad \text{(XIII-1)}$$

From the definitions of θ_1 and Φ_1 in (XIII-1), we see that

$$\Phi_1(\tau) = b(\tau)/a(\tau) .$$

Substituting (XIII-1) into equations (II-4) and (II-5), we obtain

$$\dot{\theta}_1 = -2i\alpha\cos\tau\ \Phi_1 \qquad \text{(XIII-2)}$$

and

$$\frac{i}{\varepsilon}\dot{\Phi}_1 = \Phi_1 - \frac{i\delta}{\varepsilon}\Phi_1 + \frac{2\beta}{\varepsilon}\cos\tau\ \Phi_1 + \frac{2\alpha}{\varepsilon}\cos\tau - \frac{2\alpha}{\varepsilon}\cos\tau(\Phi_1)^2 \qquad \text{(XIII-3)}$$

From Eq. (XIII-2) it follows that if Φ_1 is known, θ_1 may be found by simple quadrature. Eq. (XIII-3) has already appeared in Section VIII in connection with Techniques T3 and T4.

Similarly, if we define the functions θ_2 and Φ_2 by:

$$a(\tau) = \Phi_2(\tau)e^{\theta_2(\tau)} \ ; \quad b(\tau) = e^{\theta_2(\tau)} , \qquad \text{(XIII-4)}$$

then the differential equations for θ_2 and Φ_2 are:

$$\dot{\theta}_2 = -i(\varepsilon - i\delta) - 2i\beta\cos\tau - 2i\alpha\cos\tau\ \Phi_2 \qquad \text{(XIII-5)}$$

and

$$-\frac{i}{\varepsilon}\dot{\Phi}_2 = \Phi_2 - \frac{i\delta}{\varepsilon}\Phi_2 + \frac{2\beta}{\varepsilon}\cos\tau\,\Phi_2 - \frac{2\alpha}{\varepsilon}\cos\tau + \frac{2\alpha}{\varepsilon}\cos\tau(\Phi_2)^2 \qquad \text{(XIII-6)}$$

Once Eq. (XIII-6) is solved for Φ_2 , θ_2 is found by a simple integration.

We use Eqs. (XIII-2) and (XIII-3) to find an approximation to one of the Floquet Normal Modes. We use Eqs. (XIII-5) and (XIII-6) to find an approximation to the other linearly independent Floquet solution.

The $(1/\varepsilon)$-Solution of Equations (XIII-3) and (XIII-6)

If $1/\varepsilon$, (δ/ε), $(2\beta/\varepsilon)$ and $(2\alpha/\varepsilon)$ are all much smaller than unity, then every term in (XIII-3) is a perturbation on the term (Φ_1) . Such a perturbation is called a "singular perturbation" since the highest order derivative term is included in the perturbation terms.

Let Φ_1 be expanded according to:*

$$\Phi_1 = \sum_{n=q}^{\infty} (1/\varepsilon)\Phi_1^{(n)} \qquad \text{(XIII-7)}$$

From the indicial equation obtained by substituting (XIII-7) into Eq. (XIII-3), there are two solutions with finite values of q : one with $q = -1$ and another with $q = 1$. As mentioned previously,

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* Defining

$$\Omega = \varepsilon - i\delta + 2\beta\cos\tau$$

and rewriting Eq. (XIII-3) as

$$\Phi_1 = \frac{i}{\Omega}\dot{\Phi}_1 - \frac{2\alpha}{\Omega}\cos\tau + \frac{2\alpha}{\Omega}\cos\tau(\Phi_1)^2$$

it is tempting to seek approximations to the solutions for Φ_1 as power series expansions in $(1/\Omega)$. This approach is not recommended because it has two disadvantages:

(1) The results for $\{a(\tau);b(\tau)\}$ <u>are not</u> of the Floquet functional form.

(2) The radius of asymptotic convergence is smaller than that of the $(1/\varepsilon)$-expansions.

we consider the case where $q = 1$ and disregard the solution with $q = -1$ since this latter solution contains terms which become infinite at certain values of τ .

The general n-th order term for the $q = 1$ solution is:

$$\Phi_1^{(n)} = i\dot{\Phi}^{(n-1)} + (i\delta - 2\beta\cos\tau)\Phi_1^{(n-1)} + 2\alpha\cos\tau[-\delta_{j1} + \sum_{j=0}^{n-1} \Phi_1^{(j)}\Phi_1^{(n-1-j)}] \tag{XIII-8}$$

where $n \geq 1$ and the "delta" with subscripts is the Krönecker delta. From expressions (XIII-8) we see that $\Phi_1^{(n)}$ is determined by the $\Phi_1^{(j)}$'s where $n > j$. Furthermore, the equation for $\Phi_1^{(n)}$ is <u>not</u> a differential equation and we therefore have no flexibility in choosing boundary conditions.

The first few orders of Φ_1 are:

$$\begin{aligned} \Phi_1^{(1)} &= -2\alpha\cos\tau \\ \Phi_1^{(2)} &= 2i\alpha\sin\tau - 2\alpha(i\delta - 2\beta\cos\tau)\cos\tau \end{aligned} \tag{XIII-9}$$

Higher order corrections are easily obtained by using Eq. (XIII-8). We obtain θ_1 by substituting the results of the $(1/\varepsilon)$-expansion of Φ_1 into (XIII-2). Choosing the arbitrary constant of integration (which is equivalent to choosing the normalization), we obtain:

$$\theta_1 = i\frac{\alpha^2}{\varepsilon^2}[2\tau + \sin(2\tau)] + \frac{\alpha^2}{\varepsilon^2}\begin{bmatrix} 2\sin^2\tau - 2\delta\tau - \delta\sin(2\tau) \\ - \frac{2i\beta}{3}\sin(3\tau) - 6i\beta\sin\tau \end{bmatrix} + \ldots$$

We recover expressions for the functions $a(\tau)$ and $b(\tau)$ by using (XIII-1). Since Φ_1 contains <u>only</u> periodic terms and since θ_1 contains periodic terms and terms linear in τ, when we assemble the expressions for $a(\tau)$ and $b(\tau)$, we find that we have obtained a <u>Floquet</u> <u>Normal</u> <u>Mode</u> as a power series in $(1/\varepsilon)$. The explicit expression for this Floquet particular solution correct through second order in $(1/\varepsilon)$ is:

<u>First Mode</u>:

$$a_1 = e^{-i\mu_1\tau}\,\phi_{a1}$$
$$b_1 = e^{-i\mu_1\tau}\,\phi_{b1} \qquad \text{(XIII-10)}$$

where

$$\mu_1 = -\frac{2\alpha^2}{\varepsilon} - \frac{2i\alpha^2\delta}{\varepsilon^2} + \ldots$$

$$\phi_{a1} = \exp[\frac{i\alpha^2}{\varepsilon}\sin(2\tau) + \frac{\alpha^2}{\varepsilon^2}[2\sin^2\tau - \delta\sin(2\tau) - \frac{2i\beta}{3}\sin(3\tau) - 6i\beta\sin\tau] + \ldots]$$

$$\phi_{b1} = \phi_{a1}[-\frac{2\alpha}{\varepsilon}\cos\tau + \frac{2\alpha}{\varepsilon^2}[i\sin\tau - (i\delta - 2\beta\cos\tau)\cos\tau] + \ldots]$$

In an exactly similar manner, we find that ~~another~~ Floquet particular solution is found by again assuming a $(1/\varepsilon)$-expansion for Φ_2 :

$$\Phi_2 = \sum_{n=q}^{\infty} (1/\varepsilon)^n \, \Phi_2^{(n)} \qquad \text{(XIII-11)}$$

Substitution of the expansion (XIII-11) into Eq. (XIII-6) yields an indicial equation which admits of a solution for <u>two</u> finite values of q : $q = -1$ and $q = 1$. We again disregard the solution with $q = -1$ since we have already obtained its inverse: the solution of Φ_1 with $q = 1$. We focus on the solution to Φ_2 with $q = 1$. (The inverse of this solution was the solution to Φ_1 which we disregarded.) The general n-th order term of the $q = 1$ solution is:

$$\Phi_2^{(n)} = -i\dot{\Phi}_2^{(n-1)} + (i\delta - 2\beta\cos\tau)\Phi_2^{(n-1)} + 2\alpha\cos\tau\left[\delta_{n1} - \sum_{j=1}^{n-1} \Phi_2^{(j)} \, \Phi_2^{(n-1-j)}\right] \qquad \text{(XIII-12)}$$

where $n \geq 1$. The various $\Phi_2^{(n)}$'s are easily found by use of (XIII-12). The approximation to Φ_2 which is generated in this manner is substituted into Eq. (XIII-5) to obtain the function θ_2 . The results for Φ_2 and θ_2 are used in Eq. (XIII-4) to obtain solutions for $a(\tau)$ and $b(\tau)$. This procedure generates another

(1/ε) solution of the Floquet Form. As we will demonstrate, it is linearly independent of the solution given by (XIII-10). This second Floquet Normal Mode explicitly is:

Second Mode:

$$a_2 = e^{-i\mu_2\tau}\,\phi_{a2}$$

$$b_2 = e^{-i\mu_2\tau}\,\phi_{b2}$$

$$\mu_2 = \varepsilon - i\delta + \frac{2\alpha^2}{\varepsilon} + \frac{2i\alpha\delta}{\varepsilon^2} + \ldots$$

$$\phi_{a2} = \phi_{b2}\left[\frac{2\alpha}{\varepsilon}\cos\tau + \frac{2\alpha}{\varepsilon^2}[i\sin\tau + \cos\tau(i\delta - 2\beta\cos\tau)] + \ldots\right]$$

$$\phi_{b2} = \exp\left[-2i\beta\sin\tau - \frac{i\alpha^2}{\varepsilon}\sin(2\tau) + \frac{\alpha^2}{\beta^2}\begin{bmatrix}2\sin^2\tau + \delta\sin(2\tau) \\ + \frac{2i\beta}{3}\sin(3\tau) + 6i\beta\sin\tau\end{bmatrix} + \ldots\right]$$

(XIII-13)

Note that we really did not have to do a separate perturbation calculation to derive the second Floquet Normal Mode. Knowing the particular solution $\{a_1(\tau), b_1(\tau)\}$, we could have obtained the other, linearly independent Floquet particular solution by using (III-22). In any case, (III-22) may be used to check the algebra used in deriving (XIII-10) and (XIII-13).

The Linear Independence of the Two (1/ε)-Solutions

Using the results of Eqs. (XIII-10) and (XIII-13), the determinant

$$D(\tau) = a_1(\tau)b_2(\tau) - a_2(\tau)b_1(\tau)$$

is given by,

$$D(\tau) = \left[1 - \frac{4\alpha^2}{\varepsilon^2}\cos^2\tau - \frac{8\alpha^2}{\varepsilon^3}\cos^2\tau(i\delta - 2\beta\cos\tau) + \ldots\right] \exp\left[-i(\varepsilon - i\delta)\tau - 2i\beta\sin\tau + \frac{4\alpha^2}{\varepsilon^2}\sin^2\tau + \ldots\right]$$

Thus, $D(\tau)$ cannot vanish for sufficiently small values of $1/\varepsilon$, $(2\alpha/\varepsilon)$, $(2\beta/\varepsilon)$ and (δ/ε) .

Since $D(\tau) \neq 0$, the two solutions which we have obtained by the (1/ε)-expansions correspond to linearly independent Floquet Normal Modes.

Convergence of the (1/ε)-Expansions

To discuss the convergence of the (1/ε)-expansions, we look at the general expression for the various $\Phi_j^{(n)}$'s :

$$\Phi_j^{(n)} = \sum \frac{(2\alpha)^a \ (2\beta)^b \ \delta^c}{\varepsilon^n} f_{abc}^{(n)} (\cos\tau, \sin\tau) \qquad \text{(XIII-14)}$$

$f_{abc}^{(n)}$ is a polynomial in $\cos\tau$ and $\sin\tau$ and it is therefore bounded. a, b and c are positive integers (or zero) such that

$$a + b + c \leq n .$$

If $(1/\varepsilon)$, (δ/ε), $(2\alpha/\varepsilon)$ and $(2\beta/\varepsilon)$ are all less than unity, we expect that the coefficients

$$\frac{(2\alpha)^{a'} \; (2\beta)^{b'} \; \delta^{c'}}{\varepsilon^{n+1}}$$

from the (n+1)-th order are smaller than the coefficients

$$\frac{(2\alpha)^{a} \; (2\beta)^{b} \; \delta^{c}}{\varepsilon^{n}}$$

from the n-th order. There is no way of being sure, however, that $\Phi_j^{(n+1)}$ is always smaller than $\Phi_j^{(n)}$ for all τ and all n. We therefore expect the series to converge asymptotically. This is the general behavior of singular perturbation solutions.

We form Floquet solutions for $a(\tau)$ and $b(\tau)$ from Φ_j and θ_j $(j = 1,2)$. The function θ_j appears as an exponentiated function in the Floquet solutions and we must therefore look at its convergence.

Consider θ_j $(j = 1,2)$. From Eqs. (XIII-2) and (XIII-5) we write the expression for θ_j as:

$$\theta_j = -i[(\epsilon - i\delta)\tau + 2\beta\sin\tau]\delta_{j2} - 2i\alpha \int \cos\tau \; \Phi_j \, d\tau \qquad \text{(XIII-15)}$$

where $j = 1,2$ and δ_{j2} is the Krönecker delta. The result of carrying out the integration on the right-hand side of Eq. (XIII-15) is to obtain a function containing only terms linear in τ and periodic terms. These terms will involve products of $(1/\epsilon)$, (δ/ϵ), $(2\beta/\epsilon)$ and $(2\alpha/\epsilon)$. If the latter terms are all much less than unity, the series expression for the result of the integration is asymptotically converging. Multiplication of an asymptotically converging series by a constant, 2α, does not affect its convergence. We therefore conclude that the $(1/\epsilon)$-expansions for θ_j will asymptotically converge as long as $(1/\epsilon)$, $(2\alpha/\epsilon)$, $(2\beta/\epsilon)$ and (δ/ϵ) are all much smaller than unity.

We summarize the present discussion by saying: The $(1/\epsilon)$-expansions of the Floquet Normal Modes given by Eqs. (XIII-10) and (XIII-13) will asymptotically converge if:

$(1/\epsilon)$, (δ/ϵ), $(2\beta/\epsilon)$ and $(2\alpha/\epsilon)$ are all much less than unity.

Discussion of $(1/\epsilon)$-Expansions

As we pointed out in our statement of the quotient equations, the problem of finding solutions to the linear, homogeneous, first order equations, Eqs. (II-4) and (II-5) may be reduced to the problem of solving one, nonlinear, first order equation: either Eq. (XIII-3) or Eq. (XIII-6). The equations for Φ_j $(j = 1,2)$ are generalized Riccati equations.* Since both equations are first order, the specification of Φ_j requires <u>one</u> arbitrary constant of integration.

Consider Φ_1 . From Floquet's Theorem we write the general solution to Eq. (XIII-3) as:†

$$\Phi_1 = \frac{b(\tau)}{a(\tau)} = \frac{C_1 e^{-i\mu_1\tau}\,\phi_{b1} + C_2 e^{-i\mu_2\tau}\,\phi_{b2}}{C_1 e^{-i\mu_1\tau}\,\phi_{a1} + C_2 e^{-i\mu_2\tau}\,\phi_{a2}}$$

where C_1 and C_2 are arbitrary constants, μ_j is a constant and $\phi_{ij}(\tau) = \phi(\tau + 2\pi)$. Using the relationship between the two characteristic exponents given by Eq. (III-32), we write

$$\Phi_1 = \frac{C_1\phi_{b1} + C_2\phi_{b2}e^{-i\varepsilon\tau-\delta\tau+2i\mu_1\tau}}{C_1\phi_{a1} + C_2\phi_{a2}e^{-i\varepsilon\tau-\delta\tau+2i\mu_1\tau}} \qquad \text{(XIII-16)}$$

Inspection of Eq. (XIII-16) shows that there are <u>always</u> two periodic solutions to Eq. (XIII-3) which are periodic with periodicity 2π . These correspond to

C_1 arbitrary ; $C_2 = 0$; $\Phi_1 = \phi_{b1}/\phi_{a1}$

$C_1 = 0$; C_2 arbitrary ; $\Phi_1 = \phi_{b2}/\phi_{a2}$

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* See Ince (1956), Sec. 2.15.

† Recall that in Section III we showed that Eqs. (II-4) and (II-5) never have Form III solutions.

We call these particular solutions the Floquet particular solutions for Φ_1 since each corresponds to a ratio of Floquet Normal Mode particular solutions.

The Floquet solutions for Φ_1 are unique in that one of them may be expanded solely in terms of inverse powers of ε. The other one has an expansion in ε^1, ε^0 and all inverse powers of ε. To express all other particular solutions to Φ_1 other than the Floquet solutions, all positive and negative powers of ε are required as well as a term proportional to ε^0. Similar considerations apply to the Floquet solutions to Eq. (XIII-6).

We found one Floquet solution to Eq. (XIII-3) as a power series in $(1/\varepsilon)^n$ $n = 1,2,\ldots,\infty$. We found the inverse of the other Floquet solution to Eq. (XIII-3) as a $(1/\varepsilon)^n$ $(n = 1,2,\ldots,\infty)$ power series solution to Eq. (XIII-6).

Relationship of T8 to Usual Singular Perturbation Treatments

When ε is very large, Eqs. (XIII-7) and (XIII-11) are "stiff" equations (the coefficient of the highest order derivative term is very small). When the term $\dot{\Phi}_j$ is included in the terms taken to be the perturbation, the perturbation is said to be singular.*

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* The textbooks by Nayfeh (1973) and Cole (1968) have excellent discussions of singular perturbations. Also see, Curtiss and Hirschfelder (1952).

The solutions to stiff equations typically have the following behavior. All solutions, regardless of their boundary conditions, rapidly approach a single function as the time variable moves forward or backward. The approached solutions are called "outer solutions." The singular perturbation series usually gives an asymptotic approximation to such an "outer solution." The solution in the immediate vicinity of the boundary is called an "inner solution" and it must be found by some technique other than singular perturbation theory.

Our present treatment differs from the typical* singular perturbation problem in two respects: The first is that we never have to compute "inner solutions." The $(1/\varepsilon)$-expansion for Φ_1 asymptotically approximates one Floquet solution for Φ_1 . The $(1/\varepsilon)$-expansion of Φ_2 asymptotically approximates the <u>inverse</u> of the <u>other</u> Floquet solution for Φ_1 . We use these approximations to obtain two linearly independent Floquet solutions to (II-4) and (II-5) which may be combined to write a solution obeying <u>arbitrary</u> boundary conditions.

The second atypical aspect of Technique T8 is that although the Floquet solutions are the particular solutions which are asymptotically

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* See Cole's (1968) discussion (in Chap. 2) of an overdamped harmonic oscillator of extremely small mass as an example of a "typical" singular perturbation problem.

approached by the singular perturbation treatment, the Floquet solutions play the role of outer solutions only when $\delta \neq 0$ and $(-\delta + 2Re(i\mu_1)) \neq 0$. To demonstrate this assertion, look at the general expression for Φ_1 given by Eq. (XIII-16). (Analogous arguments can be made for Φ_2 .) Consider first the case of nonvanishing δ . When $\delta \neq 0$, the characteristic exponent, μ_1 , is in general complex and we must therefore discuss the following cases:

Case (A): $\delta \neq 0$; $(-\delta + 2Re(i\mu_1)) > 0$.

When these conditions hold, as τ gets positively large all particular solutions approach ϕ_{b2}/ϕ_{a2} . All particular solutions approach ϕ_{b1}/ϕ_{a1} for large negative values of time. In this case, therefore, the Floquet solutions are true "outer" solutions because all particular solutions approach the Floquet solutions as τ is allowed to become (positively or negatively) large.

Case (B): $\delta \neq 0$; $(-\delta + 2Re(i\mu_1)) < 0$.

The behavior of an arbitrary particular solution in this case is that it will approach either ϕ_{b1}/ϕ_{a1} or ϕ_{b2}/ϕ_{a2} as the time is allowed to get (positively or negatively) large. In particular:

$$\Phi_1 \rightarrow \phi_{b1}/\phi_{a1} \quad \text{as} \quad \tau \rightarrow \infty$$

$$\Phi_1 \rightarrow \phi_{b2}\ \phi_{a2} \quad \text{as} \quad \tau \rightarrow -\infty \ .$$

The Floquet solutions are therefore typical outer solutions in this instance.

Case (C): $\delta \neq 0$ and $(-\delta + 2Re(i\mu_1)) = 0$; or $\delta = 0$.

When either of the two above conditions are met, the term

$$(-i\varepsilon - \delta + 2i\mu_1)$$

has no real component (recall that from Chapter III, when $\delta = 0$ the characteristic exponents, μ_1 and μ_2 , are pure real).

If $(-\varepsilon + 2Re(\mu_1))$ is non-integer, from Eq. (XIII-16) we see that the Floquet particular solutions for Φ_1 are the only two particular solutions having periodicity 2π . All others (those which must have both C_1 and C_2 nonvanishing) do not have periodicity 2π . Clearly, the particular solutions which have both C_1 and C_2 nonvanishing will never have periodicity 2π no matter how far we let the time progress either in a forward or a backward direction and thus the Floquet solutions are not "outer solutions" in this instance.

If, on the other hand, $(-\varepsilon + 2Re(\mu_1))$ is an integer, all particular solutions are Floquet solutions and there is no approach to an "outer" solution.

XIV. TECHNIQUE T9: THE $(\varepsilon - i\delta)$-EXPANSION. α AND β ARBITRARY AND BOTH ε AND δ ARE MUCH LESS THAN UNITY.

Introduction

In this section we solve equations (II-4) and (II-5) by a perturbation technique which will converge when

$$\begin{array}{l}\text{both } \varepsilon \text{ and } \delta \text{ are much less than unity} \\ \text{and } \alpha \text{ and } \beta \text{ are arbitrary.}\end{array} \qquad \text{(XIV-1)}$$

The technique, which we will call "Technique T9," consists of first solving (II-4) and (II-5) when both ε and δ are set equal to zero. We take these solutions to be the zeroth order solutions and the terms proportional to ε and δ are taken to be perturbations on the zeroth order solutions. By this technique we obtain the Floquet Normal Mode Solutions. The technique which we will detail has been used by Shirley (1963) and by Series (1970), although, neither author considers nonvanishing β and δ .

We are especially interested in using this technique for the case of either α or β being much larger than unity, since, when α, β, ε and δ are all much smaller than unity we may use "Technique T5" which has already been explained in Section IX.

The General Method

If we start with (II-4) and (II-5) and let both ε and δ go to zero, the resulting equations can be exactly solved. We have already given these solutions by equations (IV-2) and (IV-3).

Let us express the solution to (II-4) and (II-5) in the form:

$$a(\tau) = F(\tau)e^{-i(\lambda_+)\sin\tau} + G(\tau)e^{-i(\lambda_-)\sin\tau}$$

$$b(\tau) = \frac{\lambda_+}{2\alpha} F(\tau)e^{-i(\lambda_+)\sin\tau} + G(\tau)\frac{\lambda_-}{2\alpha} e^{-i(\lambda_-)\sin\tau} \qquad \text{(XIV-2)}$$

where $F(\tau)$ and $G(\tau)$ are functions to be determined and (λ_+) and (λ_-) have already been defined by (IV-3). Such a choice of $a(\tau)$ and $b(\tau)$ may be considered a solution of (II-4) and (II-5) by the "variation of constants" method. Using (XIV-2) in (II-4) and (II-5) we may obtain equations for $F(\tau)$ and $G(\tau)$:

$$\dot{F} = -(i\varepsilon + \delta)\left[\frac{(\lambda_+)F}{2\sqrt{R}} + \frac{(\lambda_-)}{2\sqrt{R}} e^{2i\sqrt{R}\,\sin\tau}\, G\right] \qquad \text{(XIV-3)}$$

$$\dot{G} = (i\varepsilon + \delta)\left[\frac{(\lambda_+)F}{2\sqrt{R}} e^{-2i\sqrt{R}\,\sin\tau}\, F + \frac{(\lambda_-)G}{2\sqrt{R}}\right] \qquad \text{(XIV-4)}$$

where R is defined by

$$R = \beta^2 + 4\alpha^2$$

The coefficients of F and G in (XIV-3) and (XIV-4) are periodic with periodicity (2π) . We may therefore use Floquet's Theorem to write F and G in the following form:

$$G = \phi_G\, e^{-i\mu'\tau}\, e^{-i(\varepsilon - i\delta)\tau/2}$$

$$F = \phi_F\, e^{-i\mu'\tau}\, e^{-i(\varepsilon - i\delta)\tau/2} \qquad \text{(XIV-5)}$$

where μ' is a constant and both ϕ_G and ϕ_F are periodic functions with periodicity (2π) . The equations for ϕ_F and ϕ_G now become:

$$\dot{\phi}_G - i\mu'\phi_G - \frac{(i\varepsilon + \delta)\beta}{2\sqrt{R}}\,\phi_G - \frac{(i\varepsilon + \delta)(\lambda_+)}{2\sqrt{R}}\, e^{-2i\sqrt{R}\,\sin\tau}\phi_F = 0 \qquad \text{(XIV-6)}$$

$$\dot{\phi}_F - i\mu'\phi_F + \frac{(i\varepsilon + \delta)\beta}{2\sqrt{R}}\,\phi_F + \frac{(i\varepsilon + \delta)(\lambda_-)}{2\sqrt{R}}\, e^{2i\sqrt{R}\,\sin\tau}\,\phi_G = 0 \qquad \text{(XIV-7)}$$

At this point we can assume that μ' , ϕ_F and ϕ_G may be expanded according to

$$\mu' = \sum_{n=0}^{\infty} (i\varepsilon + \delta)^n\, \mu'^{(n)}$$

$$\phi_j = \sum_{n=0}^{\infty} (i\varepsilon + \delta)^n\, \phi_j^{(n)} \qquad j = F,G \qquad \text{(XIV-8)}$$

We can further substitute the expansions (XIV-8) into (XIV-6) and (XIV-7), match terms in like powers of $(i\varepsilon+\delta)$, to obtain a set of perturbation equations which may be solved to obtain the $\phi_j^{(n)}$'s and $\mu'^{(n)}$'s. However, it is more convenient to recast the time dependent problem into an algebraic, time-independent problem.

Transformation of (XIV-6) and (XIV-7) Into a Time-Independent Problem

To accomplish this transformation we first use Fourier's Theorem to write ϕ_G and ϕ_F as:

$$\phi_G = \sum_{j=-\infty}^{\infty} G_j \, e^{ij\tau} \; ; \quad \phi_F = \sum_{j=-\infty}^{\infty} F_j \, e^{ij\tau} \qquad \text{(XIV-9)}$$

where the G_j's and F_j's are constants. We next write $\exp[\pm 2i\sqrt{R}\,\sin\tau]$ as a Fourier series:*

$$\exp[\pm 2i\sqrt{R}\,\sin\tau] = \sum_{q=-\infty}^{\infty} J_q(2\sqrt{R})e^{\pm iq\tau} \qquad \text{(XIV-10)}$$

where $J_q(2\sqrt{R})$ is the Bessel Function of integer order q with argument $(2\sqrt{R})$.

We may now substitute the Fourier expansions (XIV-9) and (XIV-10) into equations (XIV-6) and (XIV-7) and after we group terms multiplying each and every $e^{ij\tau}$ $(j = \infty \text{ to } -\infty)$ we obtain the following

* Abramowitz and Stegun (1964), Chap. 9.

time-independent algebraic equations for the constants F_j and G_j .

$$(j - \mu')G_j - \frac{(\varepsilon - i\delta)\beta G_j}{2\sqrt{R}} - \frac{(\varepsilon - i\delta)(\lambda_+)}{2\sqrt{R}} \sum_{p=-\infty}^{\infty} J_{p-j}(2\sqrt{R})F_p = 0 \qquad \text{(XIV-11)}$$

$$(j - \mu')F_j + \frac{(\varepsilon - i\delta)\beta F_j}{2\sqrt{R}} + \frac{(\varepsilon - i\delta)(\lambda_-)}{2\sqrt{R}} \sum_{p=-\infty}^{\infty} J_{j-p}(2\sqrt{R})G_p = 0 \qquad \text{(XIV-12)}$$

In both of the above equations, the index j ranges from $-\infty$ to $+\infty$.

Restatement of (XIV-11) and (XIV-12) As A Quantum Mechanical Stationary-State Problem

In analogy with Section V, we may think of equations (XIV-11) and (XIV-12) as the following quantum mechanical problems: solve the Schrödinger Equation

$$h_F|\mu'\rangle = \mu'|\mu'\rangle \qquad \text{(XIV-13)}$$

in the orthonormal $(|F,j\rangle;|G,j\rangle)$ basis. The operator h_F may be written as

$$h_F = h_F^{(0)} + (\varepsilon - i\delta)h_F^{(1)} \qquad \text{(XIV-14)}$$

$$h_F^{(0)}|k,j\rangle = j|k,j\rangle \qquad \begin{array}{l} k = F,G \\ j = -\infty \text{ to } \infty \end{array} \qquad \text{(XIV-15)}$$

$h_F^{(1)}$ is defined by:

$$h_F^{(1)}|F,j> \;=\; \frac{\beta}{2\sqrt{R}}|F,j> + \frac{(\lambda_-)}{2\sqrt{R}} \sum_{p=-\infty}^{\infty} J_{j-p}(2\sqrt{R})\,|G,p>$$

$$h_F^{(1)}|G,j> \;=\; -\frac{\beta}{2\sqrt{R}}|G,j> - \frac{(\lambda_+)}{2\sqrt{R}} \sum_{p=-\infty}^{\infty} J_{p-j}(2\sqrt{R})\,|F,p> \qquad \text{(XIV-16)}$$

The operator h_F is non-hermitian and we have split it up into a part independent of ε and δ and into a part linearly depending on ε and δ. Once we solve the time-independent Schrödinger Equation, equation (XIV-13), we may recover the time-dependent solutions to (II-4) and (II-5). The eigenvalue, μ', is related to a Floquet Characteristic exponent, and, if $|\mu'>$ is expanded in the $(|F,j>;|G,j>)$ basis, the expansion coefficients of the basis functions correspond to the Fourier expansion coefficients of ϕ_F and ϕ_G.

Perturbation Solution to (XIV-13)

Next we split up h_F according to (XIV-14) and solve (XIV-13) by assuming that both μ' and $|\mu'>$ may be expanded according to

$$\mu' \;=\; \sum_{n=0}^{\infty} \mu'^{(n)}(\varepsilon - i\delta)^n \; ; \qquad |\mu'> \;=\; \sum_{n=0}^{\infty} (\varepsilon - i\delta)^n|\mu'^{(n)}> \qquad \text{(XIV-17)}$$

If the expansions (XIV-17) are substituted into the Schrödinger Equation, equation (XIV-13), we may obtain a set of perturbation equations, each equation of which, is proportional to certain power of $(\varepsilon - i\delta)$. For example, the zeroth order equation

$$h_F^{(0)}|\mu'^{(0)}\rangle = \mu'^{(0)}|\mu'^{(0)}\rangle \qquad \text{(XIV-18)}$$

The solution to (XIV-18) is:

$$\mu'^{(0)} = j \; ; \quad |\mu'^{(0)}\rangle = C_{F,j}^{(0)}|F,j\rangle + C_{G,j}^{(0)}|G,j\rangle \quad \text{(XIV-19)}$$

where j is any positive or negative integer or zero and $C_{F,j}^{(0)}$ and $C_{G,j}^{(0)}$ are to-be-determined constants. The problem is thus one of degenerate perturbation theory, and just as we did in Technique T5,* we shall solve it using degenerate Rayleigh-Schrödinger perturbation theory. Since the final time-dependent results for the Floquet Normal Modes are invariant to the choice of j in (XIV-19), we will choose:

$$j = 0 \; .$$

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* See Section IX of this report.

We therefore have:

$$\mu'^{(0)} = 0 \; ; \qquad |\mu'^{(0)}\rangle = C^{(0)}_{F,0}|F,0\rangle + C^{(0)}_{G,0}|G,0\rangle \qquad \text{(XIV-20)}$$

The constants, $C^{(0)}_{F,0}$ and $C^{(0)}_{G,0}$, as well as $\mu'^{(1)}$ are found from the first order perturbation equation:

$$h^{(1)}_F|\mu'^{(0)}\rangle + h^{(0)}_F|\mu'^{(1)}\rangle = \mu'^{(1)}|\mu'^{(0)}\rangle \qquad \text{(XIV-21)}$$

Multiplying (XIV-21) first by $\langle F,0|$ and then by $\langle G,0|$ we obtain

$$\left(\frac{\beta}{2\sqrt{R}} - \mu'^{(1)}\right)C^{(0)}_{F,0} - \left(\frac{\lambda_+}{2\sqrt{R}}\right)J_0(2\sqrt{R})\,C^{(0)}_{G,0} = 0$$

$$\left(\frac{\lambda_-}{2\sqrt{R}}\right)J_0(2\sqrt{R})\,C^{(0)}_{F,0} - \left(\frac{\beta}{2\sqrt{R}} + \mu'^{(1)}\right)C^{(0)}_{G,0} = 0 \qquad \text{(XIV-22)}$$

Equations (XIV-22) have a nontrivial solution if

$$\mu'^{(1)}_{\pm} = \pm \tfrac{1}{2}\sqrt{\frac{R'}{R}} \qquad \text{(XIV-23)}$$

where

$$R' = \beta^2 + [2\alpha J_0(2\sqrt{R})]^2 \; .$$

The degeneracy is therefore broken in first order and $\mu_+'^{(1)}$ will lead to one of the Floquet Normal Modes and the choice $\mu_-'^{(1)}$ will lead to the other. Since $J_0(2\sqrt{R})$ may at its largest be unity, the magnitude of $\mu_\pm'^{(1)}$ is at its largest, $\frac{1}{2}$.

Aside from normalization, the constants $C_{F,0}^{(0)}$ and $C_{G,0}^{(0)}$ are now determined since we know $\mu_\pm'^{(1)}$. Associated with the root $\mu_+'^{(1)}$ is

$$|\mu_+'^{(0)}> \;=\; |F,0> + \frac{(\beta - \sqrt{R'})|G,0>}{J_0(2\sqrt{R})(\lambda_+)} \qquad \text{(XIV-24)}$$

Associated with the root $\mu_-'^{(1)}$ is

$$|\mu_-'^{(0)}> \;=\; \frac{(\lambda_+)J_0(2\sqrt{R})}{(\beta + \sqrt{R'})}|F,0> + |G,0>$$

Let us now find the first order correction to $|\mu_+'^{(0)}>$. This correction is given by the equation

$$h_F^{(1)}|\mu_+'^{(0)}> + h_F^{(0)}|\mu_+'^{(1)}> \;=\; \mu_+'^{(1)}|\mu_+'^{(0)}> \qquad \text{(XIV-25)}$$

We may assume that $|\mu_+'^{(1)}>$ may be expanded in the basis set:

$$|\mu_+'^{(1)}> \;=\; \sum_{k,j} C_{k,j}^{(1)}|k,j> \qquad \begin{matrix} k = F,G \\ j = -\infty \text{ to } \infty \end{matrix} . \qquad \text{(XIV-26)}$$

Substituting (XIV-26) into (XIV-25), we may solve for the $C^{(1)}_{k,j}$'s to obtain

$$|\mu'^{(1)}_{+}> \; = \; C^{(1)}_{G,0}|G,0> + C^{(1)}_{F,0}|F,0>$$

$$+ \frac{(\beta - \sqrt{R'})}{2\sqrt{R}\; J_0(2\sqrt{R})} \sum_p{}' \frac{J_p(2\sqrt{R})}{p}|F,p> - \frac{(\lambda_-)}{2\sqrt{R}} \sum_p{}' \frac{(J_{-p}(2\sqrt{R})}{p}|G,p> \qquad \text{(XIV-27)}$$

where we have used a prime on the summation signs to indicate that $p = 0$ should be excluded from the summations. The coefficients multiplying $|G,0>$ and $|F,0>$ are <u>not</u> as yet completely determined even if we impose the normalization

$$<\mu'^{(0)}_{+}|\mu'^{(1)}_{+}> \; = \; 0 \qquad \text{(XIV-28)}$$

These coefficients, as well as the second order correction to μ'_+ are, however, determined from the second order perturbation equation:

$$h^{(1)}_F|\mu'^{(1)}_{+}> + h^{(0)}_F|\mu'^{(2)}_{+}> \; = \; \mu'^{(1)}_{+}|\mu'^{(1)}_{+}> + \mu'^{(2)}_{+}|\mu'^{(0)}_{+}> \qquad \text{(XIV-29)}$$

If we first multiply (XIV-29) by $<F,0|$ and then by $<G,0|$ we get the following two equations:

$$\frac{\beta}{2\sqrt{R}}\, C^{(1)}_{F,0} - \frac{(\lambda_+)}{2\sqrt{R}}\, J_0(2\sqrt{R})\, C^{(1)}_{G,0} + \frac{(\lambda_+)(\lambda_-)}{4R} \sum_j{}' \frac{(J_{-j}(2\sqrt{R}))^2}{j}$$

$$= \tfrac{1}{2}\sqrt{\frac{R'}{R}}\, C^{(1)}_{F,0} + \mu'^{(2)}_+ \tag{XIV-30}$$

$$\frac{(\lambda_-)J_0(2\sqrt{R})}{2\sqrt{R}}\, C^{(1)}_{F,0} - \frac{\beta}{2\sqrt{R}}\, C^{(1)}_{G,0} + \frac{(\lambda_-)(\beta - \sqrt{R'})}{2J_0(2\sqrt{R})\sqrt{R}} \sum_j{}' \frac{(J_j(2\sqrt{R}))^2}{j}$$

$$= \tfrac{1}{2}\sqrt{\frac{R'}{R}}\, C^{(1)}_{G,0} + \mu'^{(2)}_+ \frac{(\beta - \sqrt{R'})^2}{J_0(2\sqrt{R})(\lambda_+)} \tag{XIV-31}$$

Since for integer order Bessel functions

$$J_j = (-1)^j J_{-j} \tag{XIV-32}$$

the summations over Bessel functions which appear in (XIV-30) and (XIV-31) vanish. For the resulting equations to have a solution we find that

$$\mu'^{(2)}_+ = 0 \,. \tag{XIV-33}$$

If we further require the normalization condition given by (XIV-28), we find that

$$C^{(1)}_{F,0} = C^{(1)}_{G,0} = 0$$

We could continue this procedure to obtain approximations to (XIV-13) to any desired degree of accuracy. We, however, will stop here and summarize our first approximate solution:

First Solution

$$\mu_+' = \tfrac{1}{2}(\varepsilon - i\delta)\sqrt{\frac{R'}{R}} + (\ldots)(\varepsilon - i\delta)^3 + \ldots$$

$$|\mu_+'> = |F,0> + \frac{(\beta - \sqrt{R'})|G,0>}{(\lambda_+)J_0(2\sqrt{R})} + \frac{(\varepsilon - i\delta)(\beta - \sqrt{R'})}{2\sqrt{R}\ J_0(2\sqrt{R})} \sum_p{}' \frac{J_p(2\sqrt{R})|F,p>}{p}$$

$$- \frac{(\varepsilon - i\delta)(\lambda_-)}{2\sqrt{R}} \sum_p{}' \frac{J_{-p}(2\sqrt{R})|G,p>}{p} + (\ldots)(\varepsilon - i\delta)^2 + \ldots \qquad \text{(XIV-34)}$$

where

$$R = \beta^2 + 4\alpha^2 \ ; \quad R' = \beta^2 + [2\alpha J_0(2\sqrt{R})]^2 \ ; \quad \lambda_- = \beta - \sqrt{R}$$

In a completely analogous manner, we may obtain the solution arising from $|\mu_-^{(0)}>$. Writing μ_- accurate through $(\varepsilon - i\delta)^2$ and writing $|\mu_->$ accurate through $(\varepsilon - i\delta)$, it explicitly is:

Second Solution

$$\mu_-' = -\tfrac{1}{2}(\varepsilon - i\delta)\sqrt{\frac{R'}{R}} + (\ldots)(\varepsilon - i\delta)^3 + \ldots$$

$$|\mu_-'> = \frac{\lambda_+ J_0(2\sqrt{R})\,|F,0>}{(\beta + \sqrt{R'})} + |G,0> + \frac{(\varepsilon - i\delta)2\alpha^2}{\sqrt{R}(\beta + \sqrt{R'})} \sum_p{}' \frac{J_{-p}(2\sqrt{R})\,|G,p>}{p}$$

$$+ \frac{(\varepsilon - i\delta)\lambda_+}{2\sqrt{R}} \sum_p{}' \frac{J_p(2\sqrt{R})\,|F,p>}{p} + (\ldots)(\varepsilon - i\delta)^2 + \ldots \qquad \text{(XIV-35)}$$

where

$$\lambda_+ = \beta + \sqrt{R}$$

The Time-Dependent Floquet Normal Modes

From equations (XIV-34) and (XIV-35), we may write to solutions for $F(\tau)$ and $G(\tau)$. By use of (XIV-2), we may write two Floquet particular solutions as a power series in $(\varepsilon - i\delta)$. μ is related to μ' by: $\mu = \mu' + \tfrac{1}{2}(\varepsilon - i\delta)$. If $|\mu'>$ is expanded in the $(|F,j>;|G,j>)$ basis, the expansion coefficient of $|k,j>$ corresponds to the Fourier expansion coefficient k_j $(k = F,G)$. For notational convenience, we will write the j-th Floquet Normal Mode as

$$a_j = e^{-i\mu_j\tau}\,\phi_{aj}$$
$$b_j = e^{-i\mu_j\tau}\,\phi_{bj} \qquad \text{(XIV-36)}$$

where

$$\phi_{aj} = \phi_{Fj}\, e^{-i(\lambda_+)\sin\tau} + \phi_{Gj}\, e^{-i(\lambda_-)\sin\tau}$$

and

$$\phi_{bj} = \frac{(\lambda_+)}{2\alpha}\,\phi_{Fj}\, e^{-i(\lambda_+)\sin\tau} + \frac{(\lambda_-)}{2\alpha}\,\phi_{Gj}\, e^{-i(\lambda_-)\sin\tau}$$

The two modes may therefore be written down by utilizing the following results:

First Mode

$$\mu_1 = \tfrac{1}{2}(\varepsilon - i\delta)\left(1 + \sqrt{\frac{R'}{R}}\right) + \ldots$$

$$\phi_{F1} = 1 + \frac{(\varepsilon - i\delta)(\beta - \sqrt{R'})}{2\sqrt{R}\, J_0(2\sqrt{R})} \sum_p{}' \frac{J_p(2\sqrt{R})e^{ip\tau}}{p} + \ldots$$

$$\phi_{G1} = \frac{(\beta - \sqrt{R'})}{(\lambda_+)J_0(2\sqrt{R})} - \frac{(\varepsilon - i\delta)(\lambda_-)}{2\sqrt{R}} \sum_p{}' \frac{J_{-p}(2\sqrt{R})e^{ip\tau}}{p} + \ldots. \qquad \text{(XIV-37)}$$

Second Mode

$$\mu_2 = \tfrac{1}{2}(\varepsilon - i\delta)\left(1 - \sqrt{\frac{R'}{R}}\right) + \ldots$$

$$\phi_{F2} = \frac{(\lambda_+)J_0(2\sqrt{R})}{(\beta + \sqrt{R'})} + \frac{(\varepsilon - i\delta)(\lambda_+)}{2\sqrt{R}} \sum_p{}' \frac{J_p(2\sqrt{R})e^{ip\tau}}{p} + \ldots$$

$$\phi_{G2} = 1 + \frac{(\varepsilon - i\delta)(2\alpha^2)}{(\beta + \sqrt{R'})\sqrt{R}} \sum_p{}' \frac{J_{-p}(2\sqrt{R})e^{ip\tau}}{p} + \ldots. \qquad \text{(XIV-38)}$$

Convergence of (ε-iδ)-Expansion

The eigenfunctions of (XIV-13), may be expanded in the $(|F,j\rangle;|G,j\rangle)$ basis:

$$|\mu'\rangle = \sum_{k=F,G} \sum_{j=-\infty}^{\infty} C_{k,j}|k,j\rangle \tag{XIV-39}$$

If we use the degenerate (ε-iδ)-expansion to solve (XIV-13), we will find that the $C_{k,j}$'s may be written as

$$C_{k,j} = \sum_{n=0}^{\infty} (\varepsilon-i\delta)^n C_{k,j}^{(n)} \tag{XIV-40}$$

Each and every $C_{k,j}^{(n)}$ may be written as sums and products of terms of the form

$$\frac{\beta J_p(2\sqrt{R})}{2\sqrt{R}\, j}, \quad \frac{(\lambda_-)J_p(2\sqrt{R})}{2\sqrt{R}\, j}, \quad \frac{(\lambda_+)J_p(2\sqrt{R})}{2\sqrt{R}\, j} \tag{XIV-41}$$

where p is any integer and j is any integer except zero. j, at its smallest, has the mangitude of unity. $J_p(2\sqrt{R})$ at its largest can be unity. $\beta/2\sqrt{R}$ can at its largest be $(\frac{1}{2})$ and both $(\lambda_-)/(2\sqrt{R})$ and $(\lambda_+)/(2\sqrt{R})$ can be at largest of magnitude unity. We therefore expect the (ε-iδ)-expansion to converge as long as ε and δ are much smaller than unity regardless of the value of α and β. Because of the cumbersome nature of this expansion we will only recommend using it, however, when either α or β is much larger than unity.

XV. FOUR NUMERICAL SOLUTIONS

In the following four chapters, we discuss four methods of numerically finding the Floquet characteristic exponents. The problem has the fundamental simplification that once one of the characteristic exponents is known (call it μ_1) the other (call it μ_2) is immediately and simply known by Eq. (III-32):

$$\mu_2 = \varepsilon - i\delta - \mu_1 \qquad \text{(XV-1)}$$

Knowledge of the characteristic exponents allows us to solve Eqs. (III-35): the homogeneous linear equations for the Fourier Expansion Coefficients.

In Chapter XVI we discuss the Meadows (1962)-Ashby (1968) general method of obtaining numerical values of the characteristic exponents. We call this technique, T10. Following Meadows and Ashby, we derive a transcendental equation which involves μ and the determinant of an infinite matrix which is independent of μ and which depends only upon the parameters α, β, δ and ε. The determinant is numerically approximated and this result is used in solving the transcendental equation for a numerical approximation to μ. In Chapter XVI we also discuss how, once the values for μ

are known, the Fourier Expansion Coefficients are most simply found. Results from Chapter III are used to introduce simplifications in finding these expansion coefficients when either or both δ and β vanish. We freely draw upon results established in Chapter XVI in the chapters following it.

In Chapter XVII we discuss the Autler and Townes (1955) numerical technique: T11. This technique only applies when $\beta = 0$. We give an expression for one of the characteristic exponents in terms of two infinite continued fractions both of which depend on the characteristic exponent. Numerical iterative techniques are described which yield values for μ . The ratios of the Fourier Expansion Coefficients $(B_{j\pm1}/A_j)$ are given as μ-dependent infinite continued fractions. These may be used to obtain numerical values for the Fourier coefficients.

In Chapter XVIII, we discuss T12. In this technique we take note of the fact that when $\beta = \delta = 0$, the problem of finding the Floquet Normal Modes reduces to the problem of numerically finding an eigenvalue and an eigenvector of a real, symmetric infinite tridiagonal matrix. As Technique T12, we recommend direct computer diagonalization of some large order but finite truncation of the infinite matrix. This is an extremely fast and easy procedure when we seek eigenvalues of a real, symmetric, tridiagonal matrix.

In Chapter XIX we give Technique T13. This technique applies for arbitrary α, β, δ and ε. The heart of the technique is numerically solving Eqs. (II-4) and (II-5) to find $\{a_j'(\tau');b_j'(\tau')\}$ where, $j = 1,2$; τ' is π when $\beta = 0$ and 2π otherwise; and

$$\{a_1'(0) = 1 ; \quad b_1'(0) = 0\}$$
$$\{a_2'(0) = 0 ; \quad b_2'(0) = 1\} .$$

We use the quantities $\{a_j'(\tau');b_j'(\tau')\}$ to form a two by two matrix. Once the eigenvalues of this matrix are known, we easily find the characteristic exponents from them.

Comparison of the Four Numerical Techniques

We ask at this point: "If we must obtain a solution to Eqs. (II-4) and (II-5) in a range of the parameters which is not treated by a perturbation method, which numerical technique should be used?" The answer depends on whether or not either or both β and δ vanish.

Case (A): $\beta \neq 0$, $\delta \neq 0$

In this instance, only T10 and T13 apply. In the Autler-Townes technique we require that $\beta = 0$ and in the direct diagonalization method we require that both β and δ vanish. So, if we wish to write a computer program able to handle arbitrary values of the parameters, either T10 or T13 must be used.

In T10 the major computational hurdle is approximating an infinite order determinant. In T13 we must numerically solve complex differential equations. Since the infinite matrix in T10 has many vanishing elements, there are far fewer arithmetical steps in T10 than in T13 and T10 is therefore preferred.

Case (B): $\beta \neq 0;\ \delta = 0$

Since only T10 and T13 can handle this case, we again recommend using T10 for the reasons given in Case (A)'s discussion.

Case (C): $\beta = 0;\ \delta \neq 0$

Here, we can use either T10, T11 or T13. In computing μ , T11 involves iterations on as well successively larger truncations of infinite continued fractions. T10 only involves successively larger order truncations of a matrix and finding determinants of these matrices. There are therefore fewer arithmetical operations involved in T10 and it is the preferred technique.

Case (D): $\beta = 0;\ \delta = 0$

Here T12 is preferred since the diagonalization of a real, symmetric triadiagonal matrix is especially fast on a computer and routines for doing so are well documented and are often found as standard computer soft-ware.

XVI. TECHNIQUE T10: THE MEADOWS-ASHBY NUMERICAL SOLUTION: ε, δ, β AND α ARBITRARY. THE NUMERICAL DETERMINATION OF FOURIER EXPANSION COEFFICIENTS.

Introduction

In this section we describe the Meadows (1962) or Ashby (1968) method of numerically finding the Floquet characteristic exponents. It is a non-perturbation method in which we derive a transcendental equation for μ which involves the evaluation of the determinant of an infinite matrix which independent of μ. The exact form of the equation to be solved depends on whether δ vanishes and whether ε is almost (or exactly) equal to an even integer. We therefore must distinguish between Case (A) and Case (B).

Case (A): α, β, δ, ε Arbitrary Except That If $\delta = 0$, ε Must Not Almost (or Exactly) Equal an Even Integer.

If $\delta \neq 0$, μ may be found by:

Step A1: Evaluate the determinant of the infinite matrix $\underset{\approx}{\Delta}_1(0)$ where $\underset{\approx}{\Delta}_1(0)$ is defined in the following manner: The rows and columns of $\underset{\approx}{\Delta}_1(0)$ are ordered according to

$$\ldots A_2, B_2, A_1, B_1, A_0, B_0, A_{-1}, B_{-1}, \ldots \text{etc.}$$

and all elements of $\underset{\approx}{\Delta}_1(0)$ vanish except for

$$(\underset{\approx}{\Delta}_1(0))_{A,j;Aj} = (\underset{\approx}{\Delta}_1(0))_{B,j;B_j} = 1$$

$$(\underset{\approx}{\Delta}_1(0))_{A,j;B,j\pm1} = \frac{\alpha}{j - \frac{1}{2}(\varepsilon - i\delta)}$$

$$(\underset{\approx}{\Delta}_1(0))_{B,j;B,j\pm1} = \frac{\alpha}{j + \frac{1}{2}(\varepsilon - i\delta)} \qquad \text{(XVI-1)}$$

$$(\underset{\approx}{\Delta}_1(0))_{B,j;B,j\pm1} = \frac{\beta}{j + \frac{1}{2}(\varepsilon - i\delta)}$$

Step A2: Once $\det(\underset{\approx}{\Delta}_1(0))$ is known, μ is found by solving,

$$\sin^2[\pi(\mu - \tfrac{1}{2}(\varepsilon - i\delta))] = \sin^2[\tfrac{\pi}{2}(\varepsilon - i\delta)]\det(\underset{\approx}{\Delta}_1(0)) \qquad \text{(XVI-2)}$$

Case (B): α and β Arbitrary. $\delta = 0$ and $\varepsilon \approx N$ Where N Is Some (Positive) Even Integer.

When $\delta = 0$ and $\varepsilon \approx N$, μ is found in the following manner:

Step B1: Evaluate the determinant of the infinite matrix $\underset{\approx}{\bar{\Delta}}_1(0)$ where $\underset{\approx}{\bar{\Delta}}_1(0)$ is identical to $\underset{\approx}{\Delta}_1(0)$ except for its $(A_{N/2})$-th row and its $(B_{-N/2})$-th row. Letting $\varepsilon = N + \xi$ where ξ is by hypothesis some small or vanishing real number the matrix elements of $\underset{\approx}{\bar{\Delta}}_1(0)$ which differ from those of $\underset{\approx}{\Delta}_1(0)$ are given by:

$$(\bar{\Delta}_1(0))_{A,N/2;A,N/2} = (-1)^{N/2} \sin(\tfrac{\pi\xi}{2})$$

$$(\bar{\Delta}_1(0))_{A,N/2;B,N/2\pm 1} = -\frac{2\alpha(-1)^{N/2}\sin(\pi\xi/2)}{\xi}$$

$$(\bar{\Delta}_1(0))_{B,N/2;B,N/2} = (-1)^{N/2} \sin(\tfrac{\pi\xi}{2}) \qquad \text{(XVI-3)}$$

$$(\bar{\Delta}_1(0))_{B,-N/2;A,-N/2\pm 1} = \frac{2\alpha(-1)^{N/2}\sin(\pi\xi/2)}{\xi}$$

$$(\bar{\Delta}_1(0))_{B,-N/2;B,-N/2\pm 1} = \frac{2\beta(-1)^{N/2}\sin(\pi\xi/2)}{\xi}$$

To numerically evaluate these matrix elements, we note that:

$$\frac{\sin(\pi\xi/2)}{\xi} = \pi/2 - \frac{(\pi/2)^3\ \xi^2}{3!} + \frac{(\pi/2)^5\ \xi^4}{5!} - \dots \frac{(-1)^n\ (\pi/2)^{2n+1}\ (\xi)^{2n}}{(2n+1)!} \dots \qquad \text{(XVI-4)}$$

In the limit of ξ going to zero, expression (XVI-4) tends to $(\pi/2)$.

<u>Step B2</u>: Evaluate μ by solving the equation:

$$\sin^2[\pi(\mu - \varepsilon/2)] = \det(\bar{\Delta}_1(0)) \qquad \text{(XVI-5)}$$

In the prescriptions for finding μ which we have give above, the solution of either (XVI-2) or (XVI-5) offers no special difficulty. The major computational hurdle is in evaluating the infinite order determinants. This is done, however, by truncating $\bar{\underset{\approx}{\Delta}}_1(0)$ or $\underset{\approx}{\Delta}_1(0)$ at some high but finite order. Since many elements of the matrices vanish, efficient computer programs may be written to evaluate the required determinants. Successively higher order truncations should be done to check the convergence of this procedure.

The present method was given by Meadows in 1962. Meadows considered a general system of N first-order linear homogeneous differential equations with periodic coefficients. He made no requirements such as stipulating that the matrix of coefficients be hermitian etc. As a numerical example, he applies his technique to the Mathieu equation.

Ashby independently formulated this technique in 1968 and he is the first author to apply it to the problem of a two-state quantum system in an oscillating classical field. Ashby considered the case of non-vanishing β but did not allow the "energy" to have an imaginary component (i.e., he required $\delta = 0$). We extend Ashby's results to include non-vanishing δ and we give explicit expressions for handling the special case of $\delta = 0$ and ε equal (or almost equal) to an even integer. In the remainder of the section we prove the results given by Eqs. (XVI-2) and (XVI-5). Our method of proof is a composite of the ideas of Meadows and Ashby.

Preliminaries to the Derivation Of Eqs. (XVI-2) and (XVI-5)

Define the functions* $\sigma^+(\tau)$ and $\sigma^-(\tau)$ by

$$a(\tau) = \sigma^+(\tau) \exp[-\tfrac{i}{2}(\varepsilon - i\delta)\tau]$$
$$b(\tau) = \sigma^-(\tau) \exp[-\tfrac{i}{2}(\varepsilon - i\delta)\tau] \qquad \text{(XVI-6)}$$

Using (XVI-6) in equations (II-4) and (II-5), we obtain the differential equations for the functions σ^+ and σ^- :

$$\dot{\sigma}^+ - \tfrac{i}{2}(\varepsilon - i\delta)\sigma^+ + 2i\alpha\cos\tau\sigma^- = 0$$
$$\dot{\sigma}^- + \tfrac{i}{2}(\varepsilon - i\delta)\sigma^- + 2i\beta\cos\tau\sigma^- + 2i\alpha\cos\tau\sigma^+ = 0 \qquad \text{(XVI-7)}$$

From Floquet's theory and from Fourier's theorem, we may write the solution to Eqs. (XV-2) as

$$\sigma^+ = e^{-i\bar{\mu}\tau} \sum_{j=-\infty}^{\infty} A_j e^{ij\tau}$$
$$\sigma^- = e^{-i\bar{\mu}\tau} \sum_{j=-\infty}^{\infty} B_j e^{ij\tau} \qquad \text{(XVI-8)}$$

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* We work with the functions σ^+ and σ^- rather than the functions a and b since this allows us to avoid division by zero in the ensuing analysis.

where $\bar{\mu}$, the A_j's and the B_j's are constants. By the definition of σ^+ and σ^- in terms of the $a(\tau)$ and $b(\tau)$ in Eqs. (XVI-6), and by comparison of Eqs. (XVI-8), (III-33) and (III-34) we relate the quantity μ in (III-33) to the quantity $\bar{\mu}$ in (XVI-8) by:

$$\mu = \bar{\mu} + \tfrac{1}{2}(\varepsilon - i\delta) \qquad \text{(XVI-9)}$$

The A_j's and B_j's in (XVI-8) are exactly those which appear in Eq. (III-34). Substituting (XVI-8) into (XVI-7) we obtain two equations of the form:

$$\sum_{j=-\infty}^{\infty} C_j \exp[-i(\bar{\mu} - j)\tau] = 0$$

If these are to be valid for all values of the variable τ , then each coefficient, C_j , must be zero. Thus we obtain two sets of equations:

$$[j - \tfrac{1}{2}(\varepsilon - i\delta) - \bar{\mu}]A_j + \alpha[B_{j+1} + B_{j-1}] = 0 \qquad \text{(XVI-10)}$$

$$[j + \tfrac{1}{2}(\varepsilon - i\delta) - \bar{\mu}]B_j + \alpha[A_{j+1} + A_{j-1}] + \beta[B_{j+1} + B_{j-1}] = 0 \qquad \text{(XVI-11)}$$

Dividing Eq. (XVI-10) by $[j - \frac{1}{2}(\varepsilon - i\delta)]$ and dividing Eq. (XVI-11) by $[j + \frac{1}{2}(\varepsilon - i\delta)]$, we obtain

$$\frac{[j - \frac{1}{2}(\varepsilon - i\delta) - \bar{\mu}]}{j - \frac{1}{2}(\varepsilon - i\delta)} A_j + \frac{\alpha}{j - \frac{1}{2}(\varepsilon - i\delta)}[B_{j+1} + B_{j-1}] = 0$$

$$\frac{[j + \frac{1}{2}(\varepsilon - i\delta) - \bar{\mu}]}{j + \frac{1}{2}(\varepsilon - i\delta)} B_j + \frac{\beta}{j + \frac{1}{2}(\varepsilon - i\delta)}[B_{j+1} + B_{j-1}]$$
$$+ \frac{\alpha}{j + \frac{1}{2}(\varepsilon - i\delta)}[A_{j+1} + A_{j-1}] = 0 \tag{XVI-12}$$

Eqs. (XVI-12) can be compactly expressed by the infinite matrix equation:

$$\underset{\approx}{\Delta}\underset{\sim}{C} = 0 \tag{XVI-13}$$

where $\underset{\sim}{C}$ is the infinite column vector the elements of which are ordered:

$$\ldots, A_1, B_1, A_0, B_0, A_{-1}, B_{-1}, \ldots$$

and $\underset{\approx}{\Delta}$ is an infinite square matrix. In $\underset{\approx}{\Delta}$ we order and label the rows and columns according to

$$\ldots, A_1, B_1, A_0, B_0, A_{-1}, B_{-1}, \ldots$$

All elements of $\underset{\approx}{\Delta}$ vanish <u>except</u> for the following:

$$(\underset{\approx}{\Delta})_{A,j;A,j} = \frac{[j - \frac{1}{2}(\varepsilon - i\delta) - \bar{\mu}]}{j - \frac{1}{2}(\varepsilon - i\delta)}$$

$$(\underset{\approx}{\Delta})_{B,j;B,j} = \frac{[j + \frac{1}{2}(\varepsilon - i\delta) - \bar{\mu}]}{j + \frac{1}{2}(\varepsilon - i\delta)}$$

$$(\underset{\approx}{\Delta})_{A,j;B,j\pm1} = \frac{\alpha}{j - \frac{1}{2}(\varepsilon - i\delta)} \qquad \text{(XVI-14)}$$

$$(\underset{\approx}{\Delta})_{B,j;B,j\pm1} = \frac{\beta}{j + \frac{1}{2}(\varepsilon - i\delta)}$$

$$(\underset{\approx}{\Delta})_{B,j;A,j\pm1} = \frac{\alpha}{j + \frac{1}{2}(\varepsilon - i\delta)}$$

If Eq. (XVI-13) is to have a non-trivial solution for the vector $\underset{\sim}{C}$, the determinant of $\underset{\approx}{\Delta}$ <u>must</u> vanish. The equation which determines $\bar{\mu}$ therefore is:

$$\det(\underset{\approx}{\Delta}(\bar{\mu})) = 0 \qquad \text{(XVI-14a)}$$

Derivation of the Transcendental Equation for $\bar{\mu}$

Eq. (XVI-14a) is difficult to solve and we therefore approach the problem of determining $\bar{\mu}$ by first defining the matrix $\underset{\approx}{\Delta}_1$ which is obtained from $\underset{\approx}{\Delta}$ by dividing every row in $\underset{\approx}{\Delta}$ by its diagonal element. $\underset{\approx}{\Delta}_1$, therefore, has all its diagonal elements equalling unity. All elements of $\underset{\approx}{\Delta}_1$ vanish except for the following:

$$(\underset{\approx}{\Delta}_1)_{A,j;A,j} = (\underset{\approx}{\Delta}_1)_{B,j;B,j} = 1$$

$$\begin{aligned} (\underset{\approx}{\Delta}_1)_{A,j;B,j\pm1} &= \frac{\alpha}{j - \tfrac{1}{2}(\varepsilon - i\delta) - \bar{\mu}} \\ (\underset{\approx}{\Delta}_1)_{B,j;B,j\pm1} &= \frac{\beta}{j + \tfrac{1}{2}(\varepsilon - i\delta) - \bar{\mu}} \\ (\underset{\approx}{\Delta}_1)_{B,j;A,j\pm1} &= \frac{\alpha}{j + \tfrac{1}{2}(\varepsilon - i\delta) - \bar{\mu}} \end{aligned} \qquad \text{(XVI-15)}$$

where we label and order the rows and columns of $\underset{\approx}{\Delta}_1$ just as we labelled and ordered the rows and columns of $\underset{\approx}{\Delta}$. Clearly, $\underset{\approx}{\Delta}_1$ and $\underset{\approx}{\Delta}_1(0)$ are related by $\underset{\approx}{\Delta}_1(0) = \lim_{\bar{\mu} \to 0} (\underset{\approx}{\Delta}_1)$.

The determinants of the two matrices $\underset{\approx}{\Delta}$ and $\underset{\approx}{\Delta}_1$ are related by:

$$\det(\underset{\sim}{\Delta}) = \left[\prod_{n=-\infty}^{\infty} \left(\frac{n - \tfrac{1}{2}(\varepsilon - i\delta) - \bar{\mu}}{n - \tfrac{1}{2}(\varepsilon - i\delta)}\right)\left(\frac{n + \tfrac{1}{2}(\varepsilon - i\delta) - \bar{\mu}}{n + \tfrac{1}{2}(\varepsilon - i\delta)}\right)\right]\det(\underset{\sim}{\Delta}_1)$$

(XVI-16)

Using the infinite product:*

$$\sin Z = Z \prod_{n \neq 0} \left(1 + \frac{Z}{n\pi}\right), \quad n = -\infty \ldots +\infty$$

we find,

$$\det(\underset{\approx}{\Delta}) = \frac{\sin[\pi(\tfrac{1}{2}(\varepsilon - i\delta) - \bar{\mu})]\sin[\pi(\tfrac{1}{2}(\varepsilon - i\delta) - \bar{\mu})]\det(\underset{\approx}{\Delta}_1)}{\sin^2[\pi/2(\varepsilon - i\delta)]}$$

By using trigonometric identities, we rewrite the previous equation as:

$$\det(\underset{\approx}{\Delta}) = \left[1 - \frac{\sin^2(\bar{\mu}\pi)}{\sin^2[\pi/2(\varepsilon - i\delta)]}\right]\det(\underset{\approx}{\Delta}_1) \qquad \text{(XVI-17)}$$

Let us now study $\det(\underset{\approx}{\Delta}_1(\bar{\mu}))$ as a function of the complex variable $\bar{\mu}$. It is easy to see that $\det(\underset{\approx}{\Delta}_1(\bar{\mu}))$ is a periodic function of $\bar{\mu}$:

$$\det(\underset{\approx}{\Delta}_1(\bar{\mu} + n)) = \det(\underset{\approx}{\Delta}_1(\bar{\mu}))$$

where n is <u>any</u> positive or negative integer. This follows from the fact that the infinite matrix $\underset{\approx}{\Delta}_1(\bar{\mu})$ is identical to the infinite matrix $\underset{\approx}{\Delta}_1(\bar{\mu} + n)$.

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* See Abramowitz and Stegun (1964), Eq. 4.3.89.

By inspection of (XVI-15), it is evident that $\det(\underset{\approx}{\Delta}_1(\bar{\mu}))$ has poles at $\bar{\mu} = \pm\frac{1}{2}(\varepsilon - i\delta) + q$ where q is any positive or negative integer or zero. These poles are <u>simple</u> <u>poles</u>. This assertion is validated by noting that the function

$$f(\bar{\mu}) = (\pm\tfrac{1}{2}(\varepsilon - i\delta) + q - \bar{\mu})\det(\underset{\approx}{\Delta}_1(\bar{\mu}))$$

has no poles at $\bar{\mu} = \pm\frac{1}{2}(\varepsilon - i\delta) + q$. Multiplication of one row of a determinant by a scalar is equivalent to multiplication of the determinant itself by the same scalar. $f(\bar{\mu})$, therefore, is the determinant of the matrix obtained by multiplying the row containing the denominator $(\pm\frac{1}{2}(\varepsilon - i\delta) + q - \bar{\mu})$ by the quantity $(\pm\frac{1}{2}(\varepsilon - i\delta) + q - \bar{\mu})$. The matrix obtained in this manner (and, therefore, its determinant) has no poles at $\bar{\mu} = \pm\frac{1}{2}(\varepsilon - i\delta) + q$.

We finally note that the residue at the poles $(\pm\frac{1}{2}(\varepsilon - i\delta) + q)$ is independent of the value of the integer q . This follows immediately from the periodicity of $\det(\underset{\approx}{\Delta}_1(\bar{\mu}))$.

With the preceeding properties in mind, we write a formal expansion of $\det(\underset{\approx}{\Delta}_1(\bar{\mu}))$ as:

$$\det(\underset{\approx}{\Delta}_1(\bar{\mu})) = K_0 + \sum_{q=-\infty}^{\infty} \frac{K_A}{[\frac{1}{2}(\varepsilon - i\delta) + q - \bar{\mu}]} + \sum_{q=-\infty}^{\infty} \frac{K_B}{[q - \frac{1}{2}(\varepsilon - i\delta) - \bar{\mu}]} \tag{XVI-18}$$

where K_0, K_A, and K_B are constants. Using the fact* that

$$\sum_{q=-\infty}^{\infty} \frac{1}{q + z} = \pi \cot \pi z$$

we write,

$$\sum_{q=-\infty}^{\infty} \frac{1}{(q \pm \frac{1}{2}(\varepsilon - i\delta) - \bar{\mu})} = \pi \cos[\pi(\pm\tfrac{1}{2}(\varepsilon - i\delta) - \bar{\mu})] \tag{XVI-19}$$

Using the summation (XVI-19) in (XVI-18), we obtain:

$$\begin{aligned} \det(\underset{\approx}{\Delta}_1(\bar{\mu})) &= K_0 + \pi K_A \cot[\pi(\tfrac{1}{2}(\varepsilon - i\delta) - \bar{\mu})] + \\ &+ \pi K_B \cot[-\pi(\tfrac{1}{2}(\varepsilon - i\delta) + \bar{\mu})] \end{aligned} \tag{XVI-20}$$

We determine the expansion coefficients in (XVI-18) by considering the limit of Eq. (XVI-18) as the imaginary part of $\bar{\mu}$ goes to $\pm\infty$. When the imaginary part of $\bar{\mu}$ becomes (positively or negatively) extremely large, the off-diagonal elements of $\underset{\approx}{\Delta}_1$ tend to become very small and $\underset{\approx}{\Delta}_1$ tends towards the infinite unit matrix. In the limit, we therefore have:

$$\lim_{Im\,\bar{\mu} \to \pm\infty} [\det(\underset{\approx}{\Delta}_1(\bar{\mu}))] = 1 \tag{XVI-21}$$

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* See Jolley (1925), Eq. (450a).

If we consider the cotangent of the complex argument $(Z_r - iZ_i)$, we have

$$\cot(Z_r - iZ_i) = \frac{i[e^{Z_i} + e^{-2iZ_r}\, e^{-Z_i}]}{[e^{Z_i} - e^{-2iZ_r}\, e^{-Z_i}]}$$

Taking the limit offers no difficulty and we obtain:

$$\lim_{Z_i \to \pm\infty} [\cot(Z_r - iZ_i)] = \pm i \qquad \text{(XVI-22)}$$

If we now look at Eq. (XVI-20) and take its limit letting the imaginary part of $\bar{\mu}$ go first to $+\infty$ and then to $-\infty$, we respectively have:

$$1 = K_0 + i\pi K_A + i\pi K_B \qquad \text{(XVI-23)}$$

$$1 = K_0 - i\pi K_A - i\pi K_B \qquad \text{(XVI-24)}$$

Add (XVI-23) to (XVI-24) to find $K_0 = 1$. Subtract (XVI-23) from (XVI-22) to find $K_B = -K_A$. We rewrite (XVI-20) by using trigonometric identities and the fact that $K_B = -K_A$ and $K_0 = 1$:

$$\det(\underset{\approx}{\Delta}_1(\bar{\mu})) = 1 + 2\pi K_A\left[\frac{\sin[\frac{\pi}{2}(\varepsilon - i\delta)]\cos[\frac{\pi}{2}(\varepsilon - i\delta)]}{\sin^2[\frac{\pi}{2}(\varepsilon - i\delta)] - \sin^2(\bar{\mu}\pi)}\right] \qquad \text{(XVI-25)}$$

This equation is valid for all values of $\bar{\mu}$, and in order to evaluate the constant, K_A , let us set $\bar{\mu}$ equal to zero to obtain

$$K_A = \frac{\tan[\pi/2(\varepsilon - i\delta)]}{2\pi}[\det(\underset{\approx}{\Delta}_1(0) - 1] \qquad \text{(XVI-26)}$$

Substituting (XVI-26) and (XVI-25) into Eq. (XVI-17), we find an expression for $\det(\underset{\approx}{\Delta}(\bar{\mu}))$ in terms of $\bar{\mu}$:

$$\det(\underset{\approx}{\Delta}(\bar{\mu})) = \det(\underset{\approx}{\Delta}_1(0)) - \frac{\sin^2(\bar{\mu}\pi)}{\sin^2[\pi/2(\varepsilon - i\delta)]} \qquad \text{(XVI-27)}$$

Eq. (XVI-27) is the important result since we use it to obtain an equation for the characteristic exponents. The original Floquet problem had a solution if $\det(\underset{\approx}{\Delta}(\bar{\mu})) = 0$. Use this relation in (XVI-27) to find:

$$\sin^2(\bar{\mu}\pi) = \sin^2[\pi/2(\varepsilon - i\delta)]\det(\underset{\approx}{\Delta}_1(0)) \qquad \text{(XVI-28)}$$

If we rewrite this equation in terms of μ by using

$$\bar{\mu} = \mu - 1/2(\varepsilon - i\delta)$$

we have Eq. (XVI-2): the basic result for numerically determining the characteristic exponents when ε does not equal a positive even integer if δ vanishes.

Case of $\delta = 0$ and ε Exactly (or Almost) An Even Integer

Clearly, if $\delta = 0$ and ε is exactly or almost equal to an even integer, Eq. (XVI-28) is not useful in determining a numerical value for μ. If we let $\varepsilon = N + \xi$ where ξ is some small or vanishing real number and N is some positive even integer, then for $\delta = 0$ the $A_{N/2}$-th row of $\underset{\approx}{\Delta}_1(0)$ contains terms proportional to $(1/\xi)$. The $B_{-N/2}$-th row of $\underset{\approx}{\Delta}_1(0)$ also contains terms proportional to $(1/\xi)$. Such terms are indeterminate as ξ approaches zero and are very large for ξ very small. We must therefore patch things up.

This is easily done by noting that the right-hand side of (XVI-28) may be rewritten as

$$\det(\underset{\approx}{\bar{\Delta}}_1(0)) \qquad \text{(XVI-29)}$$

where the matrix $(\underset{\approx}{\bar{\Delta}}_1(0))$ is generated from the matrix $(\underset{\approx}{\Delta}_1(0))$ by multiplying the $A_{N/2}$-th row of $\underset{\approx}{\Delta}_1(0)$ by $\sin[\pi\varepsilon/2]$ and multiplying the $B_{-N/2}$-th row of $\underset{\approx}{\Delta}_1(0)$ by $\sin[\pi\varepsilon/2]$. Letting $\varepsilon = N + \xi$, we have

$$\sin(\frac{\pi\varepsilon}{2}) = (-1)^{N/2} \sin(\frac{\pi\xi}{2})$$

The effect of these row multiplications is to produce a right-hand side of (XVI-28) which converges for ξ going to zero. We therefore have found how to re-express Eq. (XVI-2) for the instance of $\delta = 0$ and ε being an even integer, by finding is appropriate limiting form. We have summarized the procedure to be used in this case as Steps B1 and B2 in the introduction to this chapter.

Numerical Determination of Fourier Expansion Coefficients

We now focus our attention on numerically finding the Fourier Expansion Coefficients. Our present discussion does not depend on how we numerically find μ . As usual, we write the Floquet Normal Modes as:

$$a_k = e^{-i\mu_k\tau} \sum_{j=-\infty}^{\infty} A_{jk} e^{ij\tau}$$

$$b_k = e^{-i\mu_k\tau} \sum_{j=-\infty}^{\infty} B_{jk} e^{ij\tau} \qquad \text{(XVI-30)}$$

where $k = 1$ or 2 , μ_k is constant and the A_{jk}'s and B_{jk}'s are the Fourier Expansion Coefficients. We have already derived the infinite linear homogeneous equations which determine the expansion coefficients and they are given by Eqs. (III-35).

Assume a value of μ has been found by any of the numerical techniques. Call it μ_1 . The other characteristic exponent, μ_2 , is found by

$$\mu_2 = \varepsilon - i\delta - \mu_1 \qquad \text{(XVI-31)}$$

The expansion coefficients $\{A_{j1};B_{j1}\}$ and $\{A_{j2};B_{j2}\}$ are associated with μ_1 and μ_2 respectively.

Using μ_k in Eq. (III-35) to find $\{A_{jk};B_{jk}\}$ we numerically solve Eq. (III-35) by truncating the infinite set of equations to a set of M homogeneous linear equations in M unknowns. These can be solved by well known numerical techniques. (See Wilkinson (1965), Chap. 4.) Successively larger order truncations should be taken to insure that this numerical method of approximation is converging. Care must also be taken in knowing μ to sufficient accuracy, since, if the determinant of the truncated coefficient matrix is not exceedingly small (or zero) numerical instabilities will be introduced into the problem. The expansion coefficients will in general be complex constants. We then use the same technique to find the expansion coefficients associated with the other value of μ . We do find however that if certain parameters vanish, simplifications are introduced into the problem. We therefore discuss the following four cases:

Case C1: $\beta \neq 0$; $\delta \neq 0$.

In this case the coefficients are complex. No simplifications may be introduced and Eq. (III-35) must be solved once with $\mu = \mu_1$ and again with $\mu = \mu_2$ to find $\{A_{j1};B_{j1}\}$ and $\{A_{j2};B_{j2}\}$ respectively.

<u>Case C2: $\beta = 0, \delta \neq 0$</u>.

Although the Fourier Expansion Coefficients are complex, a slight simplification will arise. If $\beta = 0$, Eq. (III-35) shows that only even B_j's are coupled to odd A_j's and only odd B_j's are coupled to even A_j's . This means that for the Fourier Expansion Coefficients associated with μ_1 we will find either (a) all odd A_j's and all even B_j's vanish, or (b) all even A_j's and all odd B_j's vanish. Except if we use the Autler-Townes Technique (T11), we do not <u>á priori</u> know whether type (a) solutions or type (b) solutions correspond to the numerically computed value of μ_1 . We will <u>á posteriori</u> find this out. In the computation of the expansion coefficients corresponding to μ_2 we will therefore know whether to assume type (a) or type (b) solutions. This knowledge will save some computational effort.

In the Autler-Townes technique (T11), we know before we compute it, whether μ_1 corresponds to type (a) or type (b) solutions. We therefore may automatically set half of the expansion coefficients equal to zero when computing them. The same is true of μ_2 and the expansion coefficients associated with it.

<u>Case C3: $\beta \neq 0, \delta = 0$</u>.

A fundamental simplification which arises in this case is that the A_{jk}'s and B_{jk}'s must be pure real. In Chapter III we showed that μ is pure real when $\delta = 0$. The matrix $\underset{\approx}{M}$ in Eq. (III-35) is pure real and therefore the A_{jk}'s and B_{jk}'s are pure real. Complex arithmetic need not be used in numerically computing them.

A further simplification arises because the A_{j2}'s and B_{j2}'s are obtained in terms of the A_{j1}'s and B_{j1}'s by:

$$A_{j2} = -\sum_{k=-\infty}^{\infty} (B_{k1}) J_{-j-k}(2\beta)$$

(XVI-32)

$$B_{j2} = \sum_{k=-\infty}^{\infty} (A_{k1}) J_{-j-k}(2\beta)$$

where $J_q(2\beta)$ is the integer order Bessel Function of order q and argument (2β) . If (2β) is small only a few terms in (XVI-32) need be retained since $J_q(2\beta)$ is given by*

$$J_q(2\beta) = (-1)^q \beta^{|q|} \sum_{k=0}^{\infty} \frac{(-\beta^2)^k}{k!(q+k)}$$

and it is therefore small for small values of (2β) .

To prove (XVI-32), we note that from Eq. (III-18), we have:

$$a_2 = -b_1^* e^{-i\varepsilon\tau} e^{-2i\beta\sin\tau}$$

(XVI-33)

$$b_2 = a_1^* e^{-i\varepsilon\tau} e^{-2i\beta\sin\tau}$$

If a_1, a_2, b_1 and b_2 are given by (XVI-30), we use the fact that $\mu_2 = \varepsilon - \mu_1$ to write:

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* Abramowitz and Stegun (1964), Eq. (9.1.10).

$$\sum_{j=-\infty}^{\infty} A_{j2}\, e^{ij\tau} = -\sum_{j=-\infty}^{\infty} B_{j1}\, e^{-ij\tau}\, e^{-2i\beta\sin\tau}$$

$$\sum_{j=-\infty}^{\infty} B_{j2}\, e^{ij\tau} = \sum_{j=-\infty}^{\infty} A_{j1}\, e^{-ij\tau}\, e^{-2i\beta\sin\tau} \qquad \text{(XVI-34)}$$

Substituting*

$$e^{-2i\beta\sin\tau} = \sum_{q=-\infty}^{\infty} J_q(2\beta)e^{-iq\tau}$$

into Eqs. (XVI-34), we obtain two equations of the form

$$\sum_{j=-\infty}^{\infty} C_j[e^{-ij\tau}] = 0$$

If these are to be valid for all values of τ, the result given by (XVI-32) must be true.

Case C4: $\beta = 0,\ \delta = 0$.

We again know that the expansion coefficients are real and in this case, the determination of the A_{j2}'s and B_{j2}'s from the A_{j1}'s and B_{j1}'s is very easy. Take the limit of Eq. (XVI-32) as β goes to zero. Using the result:

$$\lim_{\beta\to 0}[J_q(2\beta)] = \delta_{q0}\ ,$$

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* Abramowitz and Stegun (1964), Chap. 9.

we have

$$A_{j2} = -B_{-j1}$$

$$B_{j2} = A_{-j2} \qquad \text{(XVI-35)}$$

XVII. TECHNIQUE T11: THE AUTLER-TOWNES NUMERICAL SOLUTION: ε, δ AND α ARBITRARY. $\beta = 0$.

Introduction

If $\beta = 0$, we can numerically determine the characteristic exponents and the Fourier Expansion Coefficients by a technique first formulated by Autler and Townes (1955). We call the technique T11. Autler and Townes derived an expression for the characteristic exponent for the two-level system in an oscillating field. We trivially extend their work to include the case of non-vanishing δ .* Their technique involves the following steps:

Step 1: Find the characteristic exponent associated with the solution which has all odd A_j's and all even B_j's equal to zero by using the following exact expression for μ :

$$\frac{\mu}{\alpha} = -\cfrac{1}{M_1 - \cfrac{1}{M_2 - \cfrac{1}{M_3 - \cfrac{1}{M_4 - \cdots}}}} - \cfrac{1}{M_{-1} - \cfrac{1}{M_{-2} - \cfrac{1}{M_{-3} - \cfrac{1}{M_{-4} - \cdots}}}} \qquad \text{(XVII-1)}$$

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* Unfortunately, T11 cannot be extended to cover the case of non-vanishing β .

where

$$M_j = \frac{1}{\alpha}(j - \mu) \qquad j \text{ even}$$

$$M_j = \frac{1}{\alpha}(j + \varepsilon - i\delta - \mu) \qquad j \text{ odd} \qquad \text{(XVII-2)}$$

Eq. (XVII-1) gives the (in general) complex quantity μ in terms of two infinite continued fractions which themselves involve μ. As it stands, we are not able to manipulate Eq. (XVII-1) to obtain μ as an explicit function of the parameters α, ε and δ. It is, however, amenable to numerical solution and Autler and Townes report that the following algorithm has been successfully used to obtain μ.

A trial value of μ is used in (XVII-1) and the two continued fractions are evaluated with two or three denominators retained. If the sum of the two fractions does not equal the original trial value of μ, try a new value of μ between the computed value and the original trial value. Continue this procedure until the trial value and the computed value agree within some specified accuracy. Repeat this procedure using several additional denominators. When the result is unaffected by using two additional denominators, we can consider the final value of μ to be the final result.

Step 2: The value of μ from Step 1 (call it μ_1) is associated with the solution which has all odd A_j's and all even B_j's vanishing. The non-vanishing coefficients are computed from,

$$\frac{B_{j-1}}{A_j} = -M_j + \cfrac{1}{M_{j+1} - \cfrac{1}{M_{j+2} - \cfrac{1}{M_{j+3} - \cfrac{1}{M_{j+4} - \cdots}}}} \qquad \text{(XVII-3)}$$

and

$$\frac{B_{j+1}}{A_j} = -M_j + \cfrac{1}{M_{j-1} - \cfrac{1}{M_{j-2} - \cfrac{1}{M_{j-3} - \cfrac{1}{M_{j-4} - \cdots}}}} \qquad \text{(XVII-4)}$$

We are free to choose normalization and therefore the procedure is to arbitrarily set $A_0 = 1$. We find B_{-1} from (XVII-3) and we find B_1 from (XVII-4). Knowing B_1 we use (XVII-3) to find A_2 . A_{-2} is found by using the value of B_{-1} in (XVII-4), etc. This procedure is continued until we find that the coefficients generated are smaller than some predetermined magnitude. The bottleneck in the procedure is, of course, the evaluation of the infinite continued fractions which are dependent on the known value of μ . This offers, however, no great difficulty. We compute $(B_{j\pm1}/A_j)$ by first retaining, for example, two denominators. Successively retain two more denominators until the numerical value of $(B_{j\pm1}/A_j)$ does not change within some specified accuracy.

Step 3: μ_2 is simply given by

$$\mu_2 = \varepsilon - i\delta - \mu_1$$

If $\delta \neq 0$, repeat the procedure in Step 2 now choosing $B_0 = 1$ since we seek the solution with all even A_j's and all odd B_j's equal to zero. If $\delta = 0$ the second set of Fourier Expansion Coefficients are found by inspection from Eq. (XVI-35).

Derivation of T11

In what follows we derive the equations used in the Autler-Townes method. We give results in terms of the notation already introduced and we trivially extend Autler and Townes' results to include non-vanishing δ.

Starting with Eqs. (II-4) and (II-5), we set $\beta = 0$:

$$\begin{aligned} \dot{a} &= -2i\alpha\cos\tau b \\ \dot{b} &= -i(\varepsilon - i\delta) - 2i\alpha\cos\tau a \end{aligned} \qquad \text{(XVII-5)}$$

We make use of the Floquet results as well as Fourier's Theorem to write the solutions to (XVII-5) as:

$$a = e^{-i\mu\tau} \sum_{j=-\infty}^{\infty} A_j \; e^{ij\tau}$$

$$b = e^{-i\mu\tau} \sum_{j=-\infty}^{\infty} B_j \; e^{ij\tau} \qquad \text{(XVII-6)}$$

where the A_j's and B_j's are Fourier Expansion Coefficients. Substituting (XVII-6) into (XVII-5) we obtain two sets of equations for the expansion coefficients which involve the as-yet-undetermined characteristic exponent:

$$M_j A_j + B_{j-1} + B_{j+1} = 0 \qquad \text{(XVII-7)}$$

$$M_{j+1} B_{j+1} + A_j + A_{j+2} = 0 \qquad \text{(XVII-8)}$$

where

$$M_j = \frac{1}{\alpha}(j - \mu) \qquad j \text{ even}$$

$$= \frac{1}{\alpha}(j + \varepsilon - i\delta - \mu) \qquad j \text{ odd} \qquad \text{(XVII-9)}$$

If we now let

$$x_j = \frac{B_{j-1}}{A_j} \quad \text{and} \quad y_j = \frac{B_{j+1}}{A_j} \qquad \text{(XVII-10)}$$

then Eq. (XVII-7) becomes

$$M_j + x_j + y_j = 0 \qquad \text{(XVII-11)}$$

and Eq. (XVII-8) can be written in either of two forms:

$$M_{j+1} + \frac{1}{y_j} + \frac{1}{x_{j+2}} = 0 \qquad \text{(XVII-12)}$$

or

$$M_{j-1} + \frac{1}{x_j} + \frac{1}{y_{j-2}} = 0 \qquad \text{(XVII-13)}$$

From Eqs. (XVII-11) and (XVII-12), we eliminate y_j to obtain for x_j :

$$x_j = -M_j + \cfrac{1}{M_{j+1} + \cfrac{1}{x_{j+2}}} \qquad \text{(XVII-14)}$$

By iteration on Eq. (XVII-14), we have:

$$\frac{B_{j-1}}{A_j} = x_j = -M_j + \cfrac{1}{M_{j+1} - \cfrac{1}{M_{j+2} - \cfrac{1}{M_{j+3} + \cfrac{1}{x_{j+4}}}}} \qquad \text{(XVII-15)}$$

$$= -M_j + \cfrac{1}{M_{j+1} - \cfrac{1}{M_{j+2} - \cfrac{1}{M_{j+3} - \cfrac{1}{M_{j+4} - \cdots}}}}$$

This is just the expression which we wrote as Eq. (XVII-3) and which we use in the numerical determination of Fourier Expansion Coefficients. Similarly, if we eliminate x_j between Eqs. (XVII-11) and (XVII-13), we obtain y_j as:

$$y_j = -M_j + \cfrac{1}{M_{j-1} + \cfrac{1}{y_{j-2}}} \qquad \text{(XVII-16)}$$

Performing iterations on this expression we have:

$$\frac{B_{j+1}}{A_j} = y_j = -M_j + \cfrac{1}{M_{j-1} - \cfrac{1}{M_{j-2} - \cfrac{1}{M_{j-3} - \cfrac{1}{M_{j-4} - \cdots}}}} \qquad \text{(XVII-17)}$$

This is just the expression previously written as (XVII-4).

It is also easy to obtain $1/x_j$ and $1/y_j$ as infinite continued fractions. From (XVII-13) we have

$$\frac{A_j}{B_{j-1}} = \frac{1}{x_j} = -M_{j-1} - \frac{1}{y_{j-2}}$$

Combining this with Eq. (XVII-16),

$$\frac{A_j}{B_{j-1}} = -M_{j-1} + \cfrac{1}{M_{j-2} - \cfrac{1}{M_{j-3} - \cfrac{1}{M_{j-4} - \cfrac{1}{M_{j-5} - \cdots}}}} \qquad \text{(XVII-18)}$$

In an exactly similar fashion we combined Eqs. (XVII-12) and (XVII-15) to find:

$$\frac{A_j}{B_{j+1}} = -M_{j+1} + \cfrac{1}{M_{j+2} - \cfrac{1}{M_{j+3} - \cfrac{1}{M_{j+4} - \cfrac{1}{M_{j+5} - \cdots}}}} \qquad \text{(XVII-19)}$$

Since Eqs. (XVII-7) and (XVII-8) couple even A_j's with odd B_j's and vice versa, there are two linearly independent particular solutions to Eqs. (XVI-3) and (XVI-4):

First solution: All A_j's <u>even</u>; all B_j's <u>odd</u>.

Second solution: All A_j's <u>odd</u>; all B_j's <u>even</u>.

These two particular solutions correspond to the two Floquet Normal Modes.

The value of μ for the <u>first</u> particular solution (or Floquet Mode) is obtained from Eq. (XVII-11) with $j = 0$.

$$M_0 + x_0 + y_0 = 0$$

Using Eqs. (XVII-15) and (XVII-17), we obtain an expression for the characteristic exponent μ which is a sum of two infinite continued fractions both of which contain μ .

$$\frac{\mu}{\alpha} = -\cfrac{1}{M_1 - \cfrac{1}{M_2 - \cfrac{1}{M_3 - \cfrac{1}{M_4 - \cdots}}}} - \cfrac{1}{M_{-1} - \cfrac{1}{M_{-2} - \cfrac{1}{M_{-3} - \cfrac{1}{M_{-4} - \cdots}}}} \qquad \text{(XVII-20)}$$

This equation is, of course, just (XVII-1) rewritten.

The value of μ for the <u>second</u> solution (or Floquet Mode) is obtained by first setting $j = 1$ in (XVII-11) and by then making use of Eqs. (XVII-15) and (XVII-17):

$$\frac{\mu}{\alpha} = \frac{1}{\alpha}(1 + \varepsilon - i\delta) - \cfrac{1}{M_2 - \cfrac{1}{M_3 - \cfrac{1}{M_4 - \cdots}}} - \cfrac{1}{M_0 - \cfrac{1}{M_{-1} - \cfrac{1}{M_{-2} - \cdots}}} \qquad \text{(XVII-21)}$$

However, the value of μ for the second mode is most easily and quickly obtained by using Eq. (III-32) and thereby excluding the evaluation of the continued fractions in Eq. (XVII-21).

XVIII. TECHNIQUE T12. COMPUTER DIAGONALIZATION OF REAL, SYMMETRIC TRIDIAGONAL MATRIX. $\beta = \delta = 0$. ε, α ARBITRARY.

This technique is simply stated: find one eigenvalue and one eigenvector of

$$(\bar{M} - \mu I)C = 0 . \qquad \text{(XVIII-1)}$$

where, μ is the eigenvalue. C is an infinite column vector the rows of which are ordered according to

$$\ldots, A_2, B_1, A_0, B_{-1}, A_{-2}, B_{-3}, \ldots \qquad \text{(XVIII-2)}$$

I is the infinite unit matrix and $\bar{M}$ is an infinite square matrix having rows and columns ordered according to (XVIII-2). All elements of $\bar{M}$ vanish except for the following:

$$(\bar{M})_{B,j;B,j} = j + \varepsilon$$

$$(\bar{M})_{A,j;A,j} = j \qquad \text{(XVIII-3)}$$

$$(\bar{M})_{A,j;B,j\pm 1} = (\bar{M})_{B,j;A,j\pm 1} = \alpha$$

$\bar{\underset{\approx}{M}}$ is therefore real, symmetric and tridiagonal. It is, however, infinite and we approach the numerical solution of (XVIII-1) by truncating $\bar{\underset{\approx}{M}}$ and $\underset{\sim}{C}$ at some large but finite order. Because of $\bar{\underset{\approx}{M}}$'s special form, solving the truncated eigenvalue problem is an extremely easy computer problem. Wilkinson discusses this at length in Chapter 5 of his (1965) book. Because of the indeterminacy in μ, we need find only one eigenvalue and one eigenvector of (XVIII-1) to determine one of the Floquet Modes. The other mode is found by using Eq. (XV-1) with $\delta = 0$. The Fourier coefficients corresponding to the other mode are simply found by applying Eqs. (XVI-35).

We recommend this direct computer diagonalization of a matrix only for the case of $\delta = \beta = 0$ since it is only for this case that the problem is especially simple.

Derivation of Eq. (XVIII-1)

We have already derived the linear equations for the Fourier Expansion Coefficients. These are given by Eqs. (XVII-7) and (XVII-8). Multiplying these latter equations by α and then setting δ equal to zero, we obtain:

$$(j - \mu)A_j + \alpha[B_{j+1} + B_{j-1}] = 0 \qquad \text{(XVIII-4)}$$

$$(j + \varepsilon - \mu)B_j + \alpha[A_{j+1} + A_{j-1}] = 0 \qquad \text{(XVIII-5)}$$

Noting that these equations have a solution for $A_j = B_k = 0$ where j is odd and k is even, we set these coefficients equal to zero and thereby derive the matrix equations given by (XVIII-1).

XIX. TECHNIQUE T13: NUMERICAL SOLUTION OF EQS. (II-4) and (II-5) TO OBTAIN CHARACTERISTIC EXPONENTS.

Introduction

T13 is a numerical method for finding the exact values of the characteristic exponent. Shirley (1963) derived this technique for $\beta = 0 = \delta$ but it can also be used when δ and β are non-vanishing. Since the major computational hurdle is numerically solving differential equations, it is easily computer programmed since routines numerically solving differential equations are often found in standard computer soft-ware.

The basic idea in T13 is to numerically find at $\tau' = \pi$ or $\tau' = 2\pi$ the values of $\{a_1'(\tau');b_1'(\tau')\}$ and $\{a_2'(\tau');b_2'(\tau')\}$ where $\{a_j'(\tau');b_j'(\tau')\}$ $(j = 1,2)$ satisfy Eqs. (II-4) and (II-5) and obey the following initial conditions:

$$\begin{aligned} &\text{Solution 1:} \quad a_1'(0) = 1 \; ; \quad b_1'(0) = 0 \\ &\text{Solution 2:} \quad a_2'(0) = 0 \; ; \quad b_2'(0) = 1 \end{aligned} \qquad \text{(XIX-1)}$$

Solutions 1 and 2 are not in general Floquet particular solutions.

We find $\{a_j'(\tau');b_j'(\tau')\}$ by using the Runge-Kutta* or some other numerical method. We use $\{a_j'(\tau');b_j'(\tau')\}$ in finding the roots to the following secular equation

$$\det\begin{vmatrix} a_1'(\tau') - s & a_2'(\tau') \\ b_1'(\tau') & b_2'(\tau') - s \end{vmatrix} = 0$$

This determines the characteristic exponents since the roots of the secular equation are related to the characteristic exponents by:

$$s = \exp[-i\mu\tau']$$

We need only find one of the characteristic exponents because both are immediately known once <u>one</u> of them is known:

$$\mu_1 + \mu_2 = \varepsilon - i\delta \qquad \text{(XIX-2)}$$

The optimum recipe to use in obtaining the characteristic exponents depends on which (if any) parameters vanish. We therefore break the discussion into four cases. Knowing values of μ, we find the Fourier Expansion Coefficients by using the methods already discussed in Chapter XVI and we thereby numerically find the Floquet solutions.

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* See Carnahan, Luther, and Wilkes (1969), Chap. 6.

Case A: α, β, δ and ε Are All Non-Vanishing

With definitions (XIX-1) in mind, the prescription is to find by some suitable numerical technique the quantities: $a_1'(2\pi)$, $b_2'(2\pi)$, $a_2'(2\pi)$ and $b_2'(2\pi)$. These are, in general, complex quantities. The complex value of μ is found by:

$$\mu_r = \frac{1}{2\pi} \tan^{-1}[- \frac{s_i}{s_r}] \qquad \text{(XIX-3)}$$

$$\mu_i = \frac{1}{2\pi} \ell n(\sqrt{(s_r)^2 + (s_i)^2}) \qquad \text{(XIX-4)}$$

where $\mu = \mu_r + i\mu_i$, and s_r and s_i are respectively the real and imaginary components of the complex number s : $s = s_r + is_i$. s is given by:

$$s = \tfrac{1}{2}[a_1'(2\pi) + b_2'(2\pi) + [(a_1'(2\pi) + b_2'(2\pi))^2 - 4e^{-2i\varepsilon\pi} e^{-2\delta\pi}]^{1/2}] \qquad \text{(XIX-5)}$$

Use (XIX-2) to find the other value of μ .

Case B: α, ε, β Are All Non-Vanishing. $\delta = 0$

Here we merely need to know $a_1'(2\pi)$. Calling

$$a_1'(2\pi) = a_r + ia_i , \qquad \text{(XIX-6)}$$

μ is pure real and it is given by:

$$\mu = \frac{1}{2\pi} \cos^{-1}[\gamma_1 \cos(\varepsilon\pi) + (1 - (\gamma_1)^2)^{1/2} \sin(\varepsilon\pi)] \quad \text{(XIX-7)}$$

where $\gamma_1 = a_r \cos(\varepsilon\pi) - a_i \sin(\varepsilon\pi)$. Again use (XIX-2) to find the other characteristic exponent.

<u>Case C: α, ε, δ Are All Non-Vanishing. $\beta = 0$</u>

For this case, we only need to find solutions 1 and 2 (defined in Eq. (XIX-1)) at $\tau' = \pi$. Assume that we know $a_1'(\pi)$ and $b_2'(\pi)$. The complex quantity μ is defined by

$$\mu = \mu_r + i\mu_i$$

and it is computed by:

$$\mu_r = \frac{1}{\pi} \tan^{-1}[-\frac{s_i}{s_r}] \quad \text{(XIX-8)}$$

$$\mu_i = \frac{1}{\pi} \ln(\sqrt{(s_r)^2 + (s_i)^2}) \quad \text{(XIX-9)}$$

where s_r and s_i are respectively the real and imaginary components of the complex number s where

$$s = s_r + is_i$$

and,

$$s = \tfrac{1}{2}[a_1'(\pi) - b_2'(\pi) + [(a_1'(\pi) - b_2'(\pi))^2 + 4e^{-i\epsilon\pi}\, e^{-\delta\pi}]^{1/2}] \qquad \text{(XIX-10)}$$

The other characteristic exponent is most simply found by use of Eq. (XIX-2).

Case D: ϵ, α Non-Vanishing. $\delta = \beta = 0$

Here we only have to know $a_1'(\pi)$. It completely determines one of the characteristic exponents. Let us define

$$a_1'(\pi) = a_r + ia_i$$

The quantity μ is pure real and it is given by

$$\mu = \frac{1}{\pi} \cos^{-1}[\gamma_2 \sin(\epsilon\pi/2) + [1 - (\gamma_2)^2]^{1/2} \cos(\epsilon\pi/2)] \qquad \text{(XIX-11)}$$

where

$$\gamma_2 = a_r \sin(\epsilon\pi/2) + a_i \cos(\epsilon\pi/2)$$

Use Eq. (XIX-2) to find the other characteristic exponent.

Derivation of Results

The fundamental result which we use in this technique is found in Appendix A as Eq. (A-12). The result, applied to Eqs. (II-4) and (II-5), is that if we know $a_1'(2\pi)$, $b_1'(2\pi)$, $a_2'(2\pi)$ and $b_2'(2\pi)$ and if

$$s = e^{-2i\pi\mu}$$

s is given as the roots to the following secular equation:*

$$\det\begin{vmatrix} a_1'(2\pi) - s & a_2'(2\pi) \\ b_1'(2\pi) & b_2'(2\pi) - s \end{vmatrix} = 0 \qquad \text{(XIX-12)}$$

Eq. (XIX-12) has two roots (which may or may not be distinct). It is sufficient, however, to deal with only one of them since we know that the two characteristic exponents are related by Eq. (XIX-2).

We get the expressions for μ given in the introduction to this chapter from (XIX-12). Simplifications are made in the final results by using some results from Chapter III.

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* To match up the notation used here with the notation used in Eq. (A-12) make the following identifications: $n = 2$; $t_0 = 0$; $P = 2\pi$; $\hat{\phi}_{11} = a_1'$; $\hat{\phi}_{12} = a_2'$; $\hat{\phi}_{21} = b_1'$ and $\hat{\phi}_{22} = b_2'$.

Case A: ε, α, δ and β Are All Non-Vanishing

Expanding the determinant in Eq. (XIX-12), we find a quadratic equation in the quantity s . The solution for s corresponding to taking the plus sign in the quadratic formula is:

$$s = \frac{1}{2}\left[a_1'(2\pi) + b_2'(2\pi) + \left[\begin{array}{l}(a_1'(2\pi) + b_2'(2\pi))^2 \\ -4[a_1'(2\pi)b_2'(2\pi) - b_1'(2\pi)a_2'(2\pi)]\end{array}\right]^{1/2}\right] \quad \text{(XIX-13)}$$

From (III-14), we have

$$a_1'(2\pi)b_2'(2\pi) - a_2'(2\pi)b_1'(2\pi) = e^{-2i\varepsilon\pi}\, e^{-2\delta\pi} \quad \text{(XIX-14)}$$

Eq. (XIX-14) is used to simplify the expression for s given by (XIX-13). We thereby obtain the expression for s given by Eq. (XIX-5). Since we write

$$s = s_r + is_i$$

and

$$s = e^{-2i\pi(\mu_r + i\mu_i)} ,$$

we obtain the following two equations which determine μ_r and μ_i : the real and imaginary components of μ respectively:

$$s_r = e^{2\pi\mu_i} \cos(2\pi\mu_r)$$
$$s_i = -e^{2\pi\mu_i} \sin(2\pi\mu_r) \qquad \text{(XIX-15)}$$

These have the solution given by Eqs. (XIX-3) and (XIX-4).

<u>Case B: α, ε, β Are All Non-Vanishing. $\delta = 0$</u>

When δ vanishes we have the fundamental simplification that μ is pure real (see Chapter III for proof). Furthermore, by applying relations (III-18), we have

$$a_2'(2\pi) = -(b_1'(2\pi))^* e^{-2i\varepsilon\pi}$$
$$b_2'(2\pi) = (a_1'(2\pi))^* e^{-2i\varepsilon\pi} \qquad \text{(XIX-16)}$$

The secular equation, Eq. (XIX-12), is therefore simplified to

$$\det\begin{vmatrix} a_1'(2\pi) - s & -(b_1'(2\pi))^* e^{-2i\varepsilon\pi} \\ b_1'(2\pi) & (a_1'(2\pi))^* e^{-2i\varepsilon\pi} - s \end{vmatrix} = 0$$

(XIX-17)

We expand the determinant and use the fact that from Eq. (III-15) we have

$$a_1'(2\pi)(a_1'(2\pi))^* + b_1(2\pi)(b_1'(2\pi))^* = 1$$

to obtain:

$$s^2 - s(a_1'(2\pi) + (a_1'(2\pi))^* e^{-2i\varepsilon\pi}) + e^{-2i\varepsilon\pi} = 0 \quad \text{(XIX-18)}$$

Thus s depends only upon ε and $a_1'(2\pi)$. Calling

$$a_1'(2\pi) = a_r + ia_i$$

we find a solution for s as:

$$s = e^{-i\varepsilon\pi}[\gamma_1 + i(1 - (\gamma_1)^2)^{1/2}] \quad \text{(XIX-19)}$$

where

$$\gamma_1 = a_r \cos(\varepsilon\pi) - a_i \sin(\varepsilon\pi)$$

Since s is related to the characteristic exponent by

$$s = e^{-2i\mu\pi}$$

and since μ is pure real, we obtain the solution for μ given by Eq. (XIX-7).

General Consideration When β Vanishes

When β vanishes, a fundamental simplification occurs: we need carry out the numerical solution of Eqs. (II-4) and (II-5) only to $\tau' = \pi$ rather than $\tau' = 2\pi$.

To demonstrate this, consider the functions $\{c(\tau);d(\tau)\}$ which in terms of $a(\tau)$ and $b(\tau)$ are defined by:

$$\begin{aligned} c(\tau) &= a(\tau) \\ d(\tau) &= b(\tau)e^{i\tau} \end{aligned} \qquad \text{(XIX-20)}$$

From Eq. (II-4) and (II-5), we derive equations for $c(\tau)$ and $b(\tau)$:

$$\begin{aligned} \dot{c} &= -i\alpha(1 + e^{-2i\tau})d \\ \dot{d} &= -i(\varepsilon - 1 - i\delta)d - i\alpha(1 + e^{2i\tau})a \end{aligned} \qquad \text{(XIX-21)}$$

By Floquet's Theorem, there exist particular solutions to Eq. (XIX-21) of the form:

$$c_k = e^{-i\bar{\mu}_k\tau}\,\phi_{ck}(\tau)$$

$$d_k = e^{-i\bar{\mu}_k\tau}\,\phi_{dk}(\tau) \qquad \text{(XIX-22)}$$

where $k = 1,2$; $\phi_{jk}(\tau + \pi) = \phi_{jk}(\tau)$ where $j = c,d$ and $k = 1,2$; and $\bar{\mu}_k$ is a constant. We have already shown that for $\beta = 0$, one of the Floquet solutions for $\{a(\tau);b(\tau)\}$ is written

$$a_1(\tau) = e^{-i\mu_1\tau} \sum_{j=-\infty}^{\infty} A_{j1}\, e^{2ij\tau}$$

$$b_1(\tau) = e^{-i\mu_1\tau} \sum_{j=-\infty}^{\infty} B_{j1}\, e^{i(2j+1)\tau} \qquad \text{(XIX-23)}$$

The other is given by:

$$a_2(\tau) = e^{-i\mu_2\tau} \sum_{j=-\infty}^{\infty} A_{j2}\, e^{i(2j+1)\tau}$$

$$b_2(\tau) = e^{-i\mu_2\tau} \sum_{j=-\infty}^{\infty} B_{j2}\, e^{2ij\tau} \qquad \text{(XIX-24)}$$

Because of the indeterminacy in the characteristic exponents, we may write μ_2 as

$$\mu_2 - 1$$

and thereby write (XIX-24) as:

$$a_2(\tau) = e^{-i\mu_2\tau} \sum_{j=-\infty}^{\infty} A_{j2}\, e^{2i(j+1)\tau}$$

$$b_2(\tau) = e^{-i\mu_2\tau} \sum_{j=-\infty}^{\infty} B_{j2}\, e^{i(2j+1)\tau} \qquad \text{(XIX-25)}$$

From the definition of $\{c(\tau);d(\tau)\}$ in terms of $\{a(\tau);b(\tau)\}$ we see that there are two particular solutions to Eqs. (XIX-21) of the form:

$$c_1(\tau) = e^{-i\mu_1\tau} \sum_{j=-\infty}^{\infty} A_{j1}\, e^{2ij\tau}$$

$$d_1(\tau) = e^{-i\mu_1\tau} \sum_{j=-\infty}^{\infty} B_{j1}\, e^{2i(j+1)\tau} \qquad \text{(XIX-26)}$$

and

$$c_2(\tau) = e^{-i\mu_2\tau} \sum_{j=-\infty}^{\infty} A_{j2}\, e^{2i(j+1)\tau}$$

$$d_2(\tau) = e^{-i\mu_2\tau} \sum_{j=-\infty}^{\infty} B_{j2}\, e^{2i(j+1)\tau} \qquad \text{(XIX-27)}$$

Comparison of Eqs. (XIX-22), (XIX-26), and (XIX-27) shows that the characteristic exponents associated with the functions $\{c(\tau);d(\tau)\}$ are exactly those associated with the functions $\{a(\tau);b(\tau)\}$. When $\beta = 0$, therefore, we find the characteristic exponents associated with $\{a(\tau);b(\tau)\}$ by solving

$$\det\begin{vmatrix} c_1'(\pi) - s & c_2'(\pi) \\ d_1'(\pi) & d_2'(\pi) - s \end{vmatrix} = 0 \qquad \text{(XIX-28)}$$

where $s = e^{-i\mu\pi}$ and,

$$c'(0) = 1 \; ; \quad d'(0) = 0$$

$$c'(0) = 0 \; ; \quad d'(0) = 0$$

Since $c(\tau)$ and $d(\tau)$ are defined in terms of $a(\tau)$ and $b(\tau)$ by Eq. (XIX-20), we rewrite the secular equation, Eq. (XIX-28), as:

$$\det\begin{vmatrix} a_1'(\pi) - s & a_2'(\pi) \\ -b_1'(\pi) & -b_2'(\pi) - s \end{vmatrix} = 0 \qquad \text{(XIX-29)}$$

where $s = \exp[-i\mu\pi]$ and

$$a_1'(0) = 1 \; ; \quad b_1'(0) = 0$$

$$a_2'(0) = 0 \; ; \quad b_2'(0) = 1$$

Therefore, to numerically obtain the characteristic exponents when $\beta = 0$, we need only numerically solve Eqs. (II-4) and (II-5) from $\tau = 0$ to $\tau = \pi$ instead of from $\tau = 0$ to $\tau = 2\pi$.

Case C: α, ε, δ Are All Non-Vanishing. $\beta = 0$

Expanding the determinant in (XIX-29), we find s by solving:

$$s^2 - s[a_1'(\pi) - b_2'(\pi)] - a_1'(\pi)b_2'(\pi) + a_2'(\pi)b_1'(\pi) = 0 \tag{XIX-30}$$

From Eq. (III-14), we have

$$a_1'(\pi)b_2'(\pi) - a_2'(\pi)b_1'(\pi) = e^{-i\varepsilon\pi}\, e^{-\delta\pi} \tag{XIX-31}$$

This result is used to simplify Eq. (XII-29):

$$s^2 - s[a_1'(\pi) - b_2'(\pi)] - e^{-i\varepsilon\pi}\, e^{-\delta\pi} = 0 \tag{XIX-32}$$

Using the quadratic formula and taking the solution for s corresponding to the plus sign we find that s is (in general) complex and is given by the expression we have already written as Eq. (XIX-10). s and μ are complex and we therefore write:

$$s = s_r + is_i$$

$$\mu = \mu_r + i\mu_i$$

Since $s = e^{-i\mu\pi}$, we have the following equations which determine one value of μ :

$$\begin{aligned} s_r &= e^{\mu_i \pi} \cos(\mu_r \pi) \\ s_i &= -e^{\mu_i \pi} \sin(\mu_r \pi) \end{aligned} \qquad \text{(XIX-33)}$$

Eqs. (XIX-33) have the solutions we have already written in Eqs. (XIX-8) and (XIX-9).

<u>Case D: α, ε Arbitrary. $\beta = \delta = 0$</u>

In this case, we set $\delta = 0$ in Eq. (XIX-32) to find

$$s^2 - s[a_1'(\pi) - b_2'(\pi)] - e^{-i\varepsilon\pi} = 0 \qquad \text{(XIX-34)}$$

This result is further simplified by noting that from Eq. (III-18) we have:

$$b_2'(\pi) = (a_1'(\pi))^* e^{-i\varepsilon\pi} .$$

s is therefore determined by,

$$s^2 - s[a_1'(\pi) - (a_1'(\pi))^* e^{-i\varepsilon\pi}] - e^{-i\varepsilon\pi} = 0$$

The evaluation of s only requires knowledge of the first particular solution. Defining,

$$a_1'(\pi) = a_r + ia_i$$

a solution for s is:

$$s = [i\gamma_2 + [1 - (\gamma_2)^2]^{1/2}]e^{-i\varepsilon\pi/2} \qquad \text{(XIX-35)}$$

where

$$\gamma_2 = a_r \sin(\varepsilon\pi/2) + a_i \cos(\varepsilon\pi/2)$$

Since

$$s = e^{-i\mu\pi} = \cos(\mu\pi) - i \sin(\mu\pi)$$

we match real components of s and $\exp[-i\mu\pi]$ to obtain the expression for μ given by Eq. (XIX-11). A redundant expression for μ is found by equating the imaginary components of s and $\exp[-i\mu\pi]$.

APPENDIX A. SOME RESULTS CONCERNING LINEAR DIFFERENTIAL EQUATIONS WITH PERIODIC COEFFICIENTS

This appendix will be devoted to an exposition of some mathematical results concerning systems of linear, homogeneous, first order differential equations with periodic coefficients.

We will be concerned with systems of differential equations of the form:

$$\dot{x}_i(t) = \sum_{j=1}^{n} \theta_{ij}(t)x_j(t) \qquad i = 1, \ldots, n . \qquad \text{(A-1)}$$

For convenience we will let t be the independent variable and we will let a dot over a function denote the first derivative of that function with respect to t. The differential equation results in this appendix have been taken from Moulton's excellent book on differential equations,* which contains a generalization of the Poincaré-Floquet theory. We will also have cause to refer to results from linear algebra and we will use Noble's book on this subject as our reference on linear algebra.†

Before we specify that the $\theta_{ij}(t)$'s in (A-1) be periodic, let us make a few statements about the more general case of the $\theta_{ij}(t)$'s being arbitrary functions of t.

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* F. R. Moulton (1930).

† B. Noble (1969).

The broadest statement of the mathematical problem we are faced with is:

Find a set of functions $\{\bar{x}_i(t)\}$ $(i = 1, \ldots, n)$ which satisfy equations (A-1) and let these functions be such that we may fulfill the following conditions:

$$\bar{x}_i(t_0) = \bar{x}_{i0} \qquad i = 1, \ldots, n \,.$$

where t_0 is some arbitrary value of t and $\bar{x}_i(t)$ evaluated at t_0 equals some arbitrary number $\bar{x}_{i0}$. The functions, $\bar{x}_i(t)$, defined in this manner, constitute a "general solution" to equations (A-1).

Suppose we have found a set of functions which satisfies equations (A-1). Call this set $\{x_{i1}(t)\}$ $i = 1, \ldots, n$. This set of functions can be evaluated for $t = t_0$ and this set will satisfy a particular set of initial conditions, i.e. whatever the value of the functions is at $t = t_0$. This set is therefore called a "particular solution" to (A-1).

Suppose that we have found (n - 1) more particular solutions so that we now have a total of n sets of particular solutions. Call them

$$\{x_{i1}(t)\},\ \{x_{i2}(t)\},\ \ldots,\ \{x_{in}(t)\} \qquad i = 1, \ldots, n \,.$$

It is possible to define a new set of functions $\{\hat{x}_i(t)\}$ $i = 1, \ldots, n$ which is composed of linear combinations of the particular solutions. Define this new set by the following equations:

$$\hat{x}_i(t) = \sum_{j=1}^{n} C_j x_{ij}(t) \qquad i = 1, \ldots, n . \qquad \text{(A-2)}$$

The C_j's appearing in (A-2) are constants and therefore the functions $\{\hat{x}_i(t)\}$ satisfy (A-1). But, does this new set constitute a general solution to the original problem? The answer is "yes" if and only if the constants, C_j , can be chosen so that

$$\hat{x}_i(t_0) = \bar{x}_{i0} \qquad i = 1, \ldots, n .$$

where again the $\bar{x}_{i0}$ are arbitrary numbers which correspond to arbitrarily chosen initial conditions. The C_j's can be appropriately determined* if and only if the determinant, $D(t)$, does not vanish when evaluated at $t = t_0$. $D(t)$ is defined through the following expression:

$$D(t) = \det \begin{vmatrix} x_{11}(t) & x_{12}(t) & \cdots & x_{1n}(t) \\ x_{21}(t) & x_{22}(t) & \cdots & x_{2n}(t) \\ \cdots & \cdots & \cdots & \cdots \\ x_{n1}(t) & x_{n2}(t) & & x_{nn}(t) \end{vmatrix} \qquad \text{(A-3)}$$

* Noble, Theorem 7.9, p. 209.

Thus if $D(t_0) \neq 0$, it is possible to solve the algebraic problem which determines the C_j's and therefore our newly defined functions, the $\hat{x}_i(t)$'s , constitute a general solution to the problem and the functions $x_{ij}(t)$, which are the components of the $\hat{x}_i(t)$'s are said to be a "fundamental set of solutions" to the original problem.

This concept of a fundamental set is important from both a practical and a theoretical standpoint. From the practical standpoint, it is convenient to seek the fundamental solution for which $x_{ij}(t_0) = \delta_{ij}$. δ_{ij} is the Kröneker delta and it is used in defining a special fundamental set which obeys special, convenient initial conditions. Once these initial conditions are specified we could find the functions, $\{x_{ij}(t)\}$, which obey them by direct numerical integration of equations (A-1). $D(t_0)$, in this instance, is just unity and the determination of the C_j's for an arbitrary set of initial conditions is a trivial matter. It will be seen as this appendix unfolds that the concept of a fundamental set greatly facilitates the theoretical analysis of differential equations.

We need one result which will be used later. It concerns the function $D(t)$ which was defined by (A-3). It is: Theorem I: If D(t) is the determinant of a fundamental set of solutions, then,*

$$D(t) = D(t_0)\exp\left[\int_{t_0}^{t} \sum_{i=1}^{n} \theta_{ii}(t')dt'\right]$$

---

* For a proof, see Moulton, pp. 234-235.

This result tells us that $D(t)$ is finite and non-zero for all values of t for which the $\theta_{ii}(t)$ are continuous (i.e., all values of t for which the solution is defined). The result also tells us that the function $D(t)$ is the same (aside from normalization) for all of the infinitely possible fundamental sets and that this function, $D(t)$, is dependent only upon a constant times a function of the diagonal coefficients of the original equations.

We are now ready to restrict ourselves to the case of interest, namely, let the coefficients in (A-1) have periodicity P, i.e.

$$\theta_{ij}(t) = \theta_{ij}(t + P) \qquad i,j = 1, \ldots, n .$$

As an immediate consequence of the coefficients having periodicity P, we can show that if $\{x_i(t)\}$ is a solution to (A-1), then $\{x_i(t + P)\}$ is also a solution to (A-1). It is easy to demonstrate that this fact follows from the periodic nature of the coefficients in (A-1). Suppose that $\{x_i(t)\}$ satisfies (A-1). Let us now show that $\{x_i(t + P)\}$ also satisfies (A-1) by supposing it is true and then demonstrating that no inconsistencies arise. If $\{x_i(t + P)\}$ satisfies (A-1), then

$$\frac{dx_i(t + P)}{dt} = \sum_{j=1}^{n} \theta_{ij}(t)x_j(t + P) \qquad i = 1, \ldots, n .$$

Changing variables to $\tau = t + P$ we obtain: (as long as $\theta_{ij}(\tau) = \theta_{ij}(\tau - P)$)

$$\frac{dx_i(\tau)}{d\tau} = \sum_{j=1}^{n} \theta_{ij}(\tau - P)x_j(\tau) = \sum_{j=1}^{n} \theta_{ij}(\tau)x_j(\tau)$$

Thus, if $\{x_i(t)\}$ is a solution to (A-1), then $\{x_i(t + P)\}$ must also be a solution to (A-1).

Corollary

We shall now demonstrate that if $\theta_{ij}(t) = \theta_{ij}(t + P)$, the equations (A-1) always have at least one particular solution of the form:

$$x_i(t) = e^{-i\mu t} y_i(t) \qquad i = 1, \ldots, n . \qquad \text{(A-4)}$$

where μ is a constant and $y_i(t) = y_i(t + P)$.

The demonstration proceeds in two steps:

(a) The first step is to find the differential equations for the $y_i(t)$'s and to make sure that these equations are such that $\dot{y}_i(t) - \dot{y}_i(t + P) = 0$ for all i .

(b) The second step is this: we must make sure that the functions which we want to test can be expressed as appropriate linear combinations of some functions which make up a set of solutions which is known to be a fundamental set. We must therefore see if the algebraic problem of finding the linear expansion coefficients has a solution. This step, as well as step (a), will hopefully be illuminated by what follows.

We must now substitute (A-4) into (A-1) to get equations for the $y_i(t)$'s . These equations are:

$$\dot{y}_i(t) = i\mu y_i(t) + \sum_{j=1}^{n} \theta_{ij}(t) y_j(t) \qquad \text{(A-5)}$$

If, by hypothesis, $y_i(t) = y_i(t + P)$, then it must follow that:

$$\dot{y}_i(t) - \dot{y}_i(t + P) = 0 \qquad \text{(A-6)}$$

Evaluating (A-6) by using (A-5) and the relations:

$$y_i(t) = y_i(t + P) \ ; \quad \theta_{ij}(t) = \theta_{ij}(t + P)$$

we can see that (A-6) is satisfied.

To show that satisfying criteria such as (A-6) is no trivial matter, let us suppose that there is a particular solution to (A-1) of the form:

$$\{x_i(t) = e^{-i\mu t^2} y_i(t)\} \qquad i = 1, \ldots, n \qquad \text{(A-7)}$$

where μ is a constant and $y_i(t) = y_i(t + P)$. With this choice of functional form, the equations for the $y_i(t)$'s are:

$$\dot{y}_i(t) = 2i\mu t y_i(t) + \sum_{j=1}^{n} \theta_{ij}(t) y_j(t)$$

If the $y_i(t)$'s are to be periodic, then it must be true that (A-6) is obeyed. Evaluating (A-6) we find that:

$$2\mu P y_i(t) = 0 \qquad \text{for all } i \ .$$

Since P does not equal zero and not all $y_i(t) = 0$, then μ must be zero and therefore a particular solution of the form (A-7) does not exist for μ not equal to zero. This result is to be contrasted to the result we obtained by applying (A-6) to form (A-4), namely, a particular solution of form (A-4) for non-zero μ can exist (at least as far as criterion (A-6) is concerned).

We must next decide whether a solution of form (A-4) can be expressed in terms of fundamental set of solutions. We will attempt to express it in terms of the fundamental set for which $x_{ij}(t_0) = \delta_{ij}$. Call this fundamental set* $\{\hat{\phi}_{ij}(t)\}$. Thus if

$$x_{ij}(t) = \hat{\phi}_{ij}(t)$$

the $\hat{\phi}_{ij}(t)$'s satisfy (A-1) and $\hat{\phi}_{ij}(t_0) = \delta_{ij}$. If $\{x_i(t) = e^{-i\mu t} y_i(t)\}$ is to be expressed in terms of $\{\hat{\phi}_{ij}(t)\}$, then it must be true that

$$y_i(t) = e^{i\mu t} \sum_{j=1}^{n} C_j \hat{\phi}_{ij}(t) \qquad i = 1, \ldots, n . \qquad \text{(A-8)}$$

where the C_j's are constants. By hypothesis,

$$y_i(t + P) - y_i(t) = 0 \qquad i = 1, \ldots, n . \qquad \text{(A-9)}$$

Substituting (A-8) into (A-9), we get the n equations

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* These $\hat{\phi}$'s are not to be confused with the "uncapped" ϕ's in the main body of the report.

$$e^{i\mu(t+P)} \sum_{j=1}^{n} C_j \hat{\phi}_{ij}(t + P) - e^{i\mu t} \sum_{j=1}^{n} C_j \hat{\phi}_{ij}(t) = 0$$

$$i = 1, \ldots, n \;. \qquad \text{(A-10)}$$

If we require that $t = t_0$ and define $s = e^{-i\mu P}$, we can write (A-10) as (A-11) if we utilize the following property of the fundamental set: $\hat{\phi}_{ij}(t_0) = \delta_{ij}$.

$$\sum_{j=1}^{n} C_j [\hat{\phi}_{ij}(t_0 + P) - s\delta_{ij}] = 0 \qquad i = 1, \ldots, n \;. \qquad \text{(A-11)}$$

(A-11) is the equation for the C_j's which must be satisfied. If a solution to (A-11) exists, then we can express our assumed functional form of solution in terms of a fundamental set and thus our assumed form of solution is indeed a solution. (A-11) is nothing but an eigenvalue-eigenvector problem and, as is well known,* there is a solution to (A-11) if and only if the following determinant vanishes:

$$\det \begin{vmatrix} \hat{\phi}_{11}(t_0 + P) - s & \hat{\phi}_{12}(t_0 + P) & \cdots & \hat{\phi}_{1n}(t_0 + P) \\ \hat{\phi}_{21}(t_0 + P) & \hat{\phi}_{22}(t_0 + P) - s & \cdots & \hat{\phi}_{2n}(t_0 + P) \\ \cdot \quad \cdot \quad \cdot & \cdot \quad \cdot \quad \cdot & \cdots & \cdot \quad \cdot \quad \cdot \\ \cdot \quad \cdot \quad \cdot & \cdot \quad \cdot \quad \cdot & \cdots & \cdot \quad \cdot \quad \cdot \\ \hat{\phi}_{n1}(t_0 + P) & \hat{\phi}_{n2}(t_0 + P) & \cdots & \hat{\phi}_{nn}(t_0 + P) - s \end{vmatrix}$$

(A-12)

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* Noble, Chapter 9.

s is to be chosen by expanding the determinant and thereby obtaining a polynomial in s^n. If s is set equal to a root of this polynomial, (A-12) vanishes. The lead term in this polynomial is, of course, s^n. The coefficient of s^0 is just the determinant* of the $n \times n$ matrix which has as its i,j-th element $\hat{\phi}_{ij}(t_0 + P)$. But this matrix is just a matrix of a fundamental set of solutions and therefore its determinant can never be zero or infinite. (See Theorem I and the discussion which follows it.) Since the coefficients of the terms in $s^m (m = 1, \ldots, n - 1)$ are composed of sums of the products of various $\hat{\phi}_{ij}(t_0 + P)$'s, from Theorem I we know that these coefficients can never be infinite (it is possible, however, to have them equal to zero). Thus the characteristic polynomial equation is of the form:

$$s^n + (\text{finite terms in } s^{n-1}, \ldots, s^1) +$$
$$(\text{a number not equal to zero or infinity})$$

Thus s can itself never be zero or infinity. So then, there must be a finite, non-zero s such that (A-11) can be solved for the C_j's. This of course means that what we set out to demonstrate is indeed true, namely, there does indeed exist a particular solution to (A-1) of the form given by (A-4).

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* Noble, Theorem 9.1, p. 280.

Corollary

Note also that knowledge of s does not completely determine μ. Suppose that we have values of μ and s (call them μ_1 and s_1 respectively) such that $s_1 = e^{-i\mu_1 P}$ is satisfied. If we define a new μ, call it μ', by $\mu' = \mu_1 + \frac{2n\pi}{P}$ (n = zero or any integer), then $s_1 = e^{-i\mu' P}$ is also satisfied. Thus μ is not determined up to an additive factor of $\frac{2n\pi}{P}$. However, this in no way changes our result since if we say that $\{e^{-i\mu_1 t} y_i(t)\}$ is a solution which has the form of periodic functions multiplied by a linear exponential term, then $\{e^{-i(\mu_1 + \frac{2n\pi}{P})t} y_i(t)\}$ is also a solution which has the form of periodic functions multiplied by a linear exponential term. We can therefore ignore this indeterminacy in μ.

The crucial point in the argument that our supposed solutions exist was the existence of a non-zero, finite root to the characteristic polynomial equation. But, if we have one such root to the n-th degree polynomial, we must necessarily have a total of n such roots (some of which may be repeated). We will now direct our attention to the consequence of the characteristic polynomial's having n roots. We will limit ourselves to the following two cases:

(a) all n roots are distinct.

(b) $(n - 2)$ roots are distinct and one root is doubly degenerate.

We could treat the more general case of the number of distinct roots being arbitrary and the number of repeated roots as well as their degeneracy being arbitrary, but since the important features of the general case are displayed in this restricted case of one double degeneracy, we will just treat cases (a) and (b).*

Case (b) must actually be broken up into two subcases, since, a doubly degenerate eigenvalue may have only one linearly independent eigenvector associated with it, or, it may have two linearly independent eigenvectors associated with it.** If there are two linearly independent eigenvectors associated with the root s_{n-1}, (call this case (b-1)), then if we form the determinant (A-12) with s set equal to s_{n-1}, all first minors will be equal to zero. If there is only one linearly independent eigenvector associated with the root s_{n-1}, (call this case (b-2)), then if we form the determinant (A-12) with s set equal to s_{n-1}, there will be at least one first minor which will not be equal to zero.

To tie up this appendix with the two-level system and the main body of the report, we will note at this point that case (a) yields what we have called "Form I" solutions (see (III-4) and (III-5)). Case (b-1) gives rise to the "Form II" solutions (equations (III-7) and (III-8)). Case (b-2) will correspond to the "Form III" solutions which are given by equations (III-10) and (III-11).

For case (a), we can write the following theorem: <u>Theorem II</u>: <u>If (A-12) has n distinct roots, then there are n solutions to (A-1) of the form:</u>

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*The general case is treated in Moulton, Chapter 17.

**Noble, pp. 349-351.

$$\{\tilde{x}_{ik}(t) = e^{-i\mu_k t} y_{ik}(t)\} \qquad i,k = 1, \ldots, n \; .$$

The indices are such that $\tilde{x}_{ik}$ is the i-th function in the k-th solution. μ_k is a constant and the k-th μ is distinct from all other μ's and $y_{ik}(t) = y_{ik}(t + P)$ $(i,k = 1, \ldots, n)$. The set $\{\tilde{x}_{ik}(t)\}$ is a fundamental set of solutions to (A-1). The k-th solution may be called the k-th Floquet or normal mode.

The application of this theorem to the two-level problem is this: one possible functional form of the solutions to (II-4) and (II-5) is what we have called "Form I" and have written in equations (III-4) and (III-5).

This theorem is not difficult to prove. The fact that there are n solutions of the desired form follows from the hypothesis that (A-12) has n distinct roots. Order these roots as $\{s_1, s_2, \ldots, s_n\}$. Since there are n distinct values of s_k , there must be a value of μ_k associated with each s_k such that the μ_k's are distinct and no two differ by $\frac{2\pi n}{P}$ (n any integer or zero). Also associated with the root, s_k , is an eigenvector $(C_{1k}, C_{2k}, \ldots, C_{nk})$. The root and its eigenvector are related by equation (A-13) which is just equation (A-11) rewritten for the k-th root and its eigenvector.

$$\sum_{j=1}^{n} C_{jk}[\hat{\Phi}_{ij}(t + P) - \delta_{ij}s_k] = 0 \qquad i = 1, \ldots, n \; . \quad \text{(A-13)}$$

Since the C_{jk}'s express a solution of the desired form in terms of a fundamental set, it follows that we have n such solutions. They explicitly are:

$$\text{the first} \quad \{\tilde{x}_{i1}(t) = e^{-i\mu_1 t} y_{i1}(t) = \sum_{j=1}^{n} C_{j1}\hat{\phi}_{ij}(t)\} \quad i = 1, \ldots, n$$

$$\text{the second} \quad \{\tilde{x}_{i2}(t) = e^{-i\mu_2 t} y_{i2}(t) = \sum_{j=1}^{n} C_{j2}\hat{\phi}_{ij}(t)\} \quad i = 1, \ldots, n$$

$$\text{the n-th} \quad \{\tilde{x}_{in}(t) = e^{-i\mu_n t} y_{in}(t) = \sum_{j=1}^{n} C_{jn}\hat{\phi}_{ij}(t)\} \quad i = 1, \ldots, n \qquad \text{(A-14)}$$

But now we ask, "Do the $x_{ij}(t)$'s form a fundamental set of solutions?" We want a "yes" answer to this question and we get it by forming the matrix $\underset{\approx}{X}(t_0)$ (where $(\underset{\approx}{X}(t_0))_{ij} = \tilde{x}_{ij}(t_0)$) and by then showing that its determinant is non-zero. By the discussion preceeding Theorem I, we know that if $\det|X(t_0)| \neq 0$, then the $\tilde{x}_{ij}(t)$'s are a fundamental set of solutions. Knowing that the $\hat{\phi}_{ij}(t)$'s have been defined so that $\hat{\phi}_{ij}(t\ ) = \delta_{ij}$, we can use (A-14) to find that $(\underset{\approx}{X}(t_0))_{ij} = C_{ij}$. Thus the j-th column of $\underset{\approx}{X}(t_0)$ is just the eigenvector associated with the j-th root of (A-12). The columns of $\underset{\approx}{X}(t_0)$ are therefore linearly independent because of the fact that the eigenvectors of a $n \times n$ matrix which has n distinct eigenvalues are linearly independent.* Because the determinant of a matrix with

* Noble, Theorem 9.3, p. 281.

linearly independent columns can never vanish, we have the result that $\det|\underset{\sim}{X}(t_0)| \neq 0$ and therefore Theorem II stands confirmed.

Example AI:

In order to illustrate Theorem II, let us consider an example of a simple system to which it applies. This example is included at this particular juncture both to clarify the method of demonstration we have used and to clarify the notation used in the method. Let the system be:

$$\begin{aligned} \dot{x}_1(t) &= \cos t \; x_1(t) + \alpha x_2(t) \\ \dot{x}_2(t) &= -\alpha x_1(t) + \cos t \; x_2(t) \end{aligned} \tag{A-15}$$

Let α be a constant not equal to [illegible] n equal to zero or any integer).

To solve this system of equations we can use Kamke's* prescription for solving equations of this type, or we can simply note that if we let

$$x_1 = x_1' \exp[\sin t], \quad x_2 = x_2' \exp[\sin t],$$

(A-15) becomes

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* Kamke (1943), p. 611, Vol. 1.

$$\dot{x}_1' = \alpha x_2' \text{ and } \dot{x}_2' = -\alpha x_1' .$$

We therefore have

$$\ddot{x}_1' + \alpha^2 x_1' = 0$$

which is easily solved by elementary methods to yield the two solutions for x_1 and x_2 which are given by (A-16).

$$\begin{aligned} &\text{solution I} \quad \{\cos(\alpha t)e^{\sin t} \ ; \ -\sin(\alpha t)e^{\sin t}\} \\ &\text{solution II} \quad \{\sin(\alpha t)e^{\sin t} \ ; \ \cos(\alpha t)e^{\sin t}\} \end{aligned} \qquad \text{(A-16)}$$

That these solutions form a fundamental set may be easily demonstrated by using the definition in (A-3) to form $D(t)$:

$$D(t) = \exp[2\sin t]$$

$D(t)$ can never equal zero, thus (A-16) forms a fundamental set and, for $t_0 = 0$, the fundamental matrix of these functions is the unit matrix. We can therefore make the following identifications:

$$\hat{\phi}_{11}(t) = \cos(\alpha t)e^{\sin t} \qquad \hat{\phi}_{12}(t) = \sin(\alpha t)e^{\sin t}$$

$$\hat{\phi}_{21}(t) = -\sin(\alpha t)e^{\sin t} \qquad \hat{\phi}_{22}(t) = \cos(\alpha t)e^{\sin t}$$

The notation is such that if we were to arrange the $\hat{\phi}$ functions into a matrix, the i,j-th $\hat{\phi}$ would be the i-th function in the j-th solution. According to what has gone before, to see whether we have a solution of the $e^{-i\mu t}y(t)$ form, we must find the roots of (A-12). P for this example is 2π , and, as we have already said, t_0 is taken to equal zero. We therefore have:

$$\det \begin{vmatrix} \cos(2\pi\alpha) - s & \sin(2\pi\alpha) \\ -\sin(2\pi\alpha) & \cos(2\pi\alpha) - s \end{vmatrix} = 0 \qquad \text{(A-17)}$$

(A-17) has the solution $s_{\pm} = \exp[\pm 2i\pi\alpha]$. Since $s = \exp[-i\mu P]$, we have two values of μ not differing by an integer or zero and we therefore expect two solutions of the $e^{-i\mu t}y(t)$ form which will form a fundamental set of solutions. If we call $\mu_1 = -\alpha$ and $\mu_2 = \alpha$, it can be easily shown that associated with μ_1 is the eigenvector

$$(1,i) = (C_{11},C_{21})$$

Associated with μ_2 is the eigenvector

$$(1,-i) = (C_{12},C_{22})$$

Using the notation of (A-14) and the results so far obtained in this example, we can explicitly write the Floquet Normal Mode Solutions:

$$\{\tilde{x}_{11}(t) = e^{i\alpha t}e^{\sin t}; \quad \tilde{x}_{21}(t) = ie^{i\alpha t}e^{\sin t}\}$$
$$\{\tilde{x}_{12}(t) = e^{-i\alpha t}e^{\sin t}; \quad \tilde{x}_{22}(t) = -ie^{-i\alpha t}e^{\sin t}\} \qquad \text{(A-18)}$$

We can make the following identifications for this simple example:

$$\mu_1 = -\mu_2 = -\alpha \ ; \quad y_{11}(t) = y_{12}(t) = -iy_{21}(t) = iy_{22}(t) = e^{\sin t}$$

That the solutions of (A-18) form a fundamental set may be demonstrated by evaluating $D(t)$. It explicitly is:

$$D(t) = -2ie^{2\sin t}$$

It can be easily seen that $D(t)$ can never equal zero, and therefore, the Floquet Normal Mode Solutions are a fundamental set of solutions. This concludes the discussion of the example.

We can now proceed to consider case (b-1). Consideration of (b-1), leads to the following theorem which we are calling Theorem III. The application of this theorem to the two-level system is this: there is the possibility of having a solution of "Form II", where, "Form II" is given by equations (III-7) and (III-8). These equations can be found in the main body of the report. Theorem III: If (A-12) has only $(n - 1)$ distinct roots because the $(n - 1)$-th root is doubly degenerate and if there exist two linearly independent eigenvectors associated with the doubly degenerate root, s_{n-1} , then there are $(n - 1)$ solutions of the form:

$$\{\tilde{x}_{ik}(t) = e^{-i\mu_k t} y_{ik}(t)\} \qquad \begin{matrix} i = 1, \ldots, n \\ k = 1, \ldots, n-1 \end{matrix} \qquad \text{(A-19)}$$

<u>and, there is an additional solution of the form</u>

$$\{\tilde{x}_{in}(t) = e^{-i\mu_{n-1} t} y_{in}(t)\} \qquad i = 1, \ldots, n \ . \qquad \text{(A-20)}$$

The μ's are constants and there is a total of $(n - 1)$ distinct μ's not differing by $\frac{2\pi k}{P}$ (k equals to zero or any integer). For all $y_{ik}(t)$'s it is true that

$$y_{ik}(t) = y_{ik}(t + P) \qquad i,k = 1, \ldots, n \ .$$

The set of solutions composed of solutions (A-19) together with solution (A-20) forms a fundamental set of solutions to (A-1).

The proof of Theorem III is simple. In outline, it consists of realizing that since we can find $(n - 1)$ eigenvalues with n associated eigenvectors for (A-12), we can get the n solutions given by (A-19) and (A-20). Since the eigenvectors associated with the degenerate root are linearly independent of each other and since eigenvectors of distinct roots are also linearly independent of each other, all n eigenvectors taken together form a linearly independent set of vectors. Utilization of the same chain of reasoning we used in discussing Theorem II tells us that (A-19) and (A-20) taken together form a fundamental set of solutions to (A-1).

Example A2:

A simple example of a non-trivial problem which has the type of solution described by Theorem III is the following

$$\begin{aligned} \dot{x}_1(t) &= \alpha x_1(t) + \cos t \, x_2(t) \\ \dot{x}_2(t) &= -\cos t \, x_1(t) + \alpha x_2(t) \end{aligned} \qquad \text{(A-21)}$$

Let α be a non-zero constant not equal to im (m any integer or zero). The solution is obtain by using Kamke's* prescription. His prescription directly yields a set of fundamental solutions which, when evaluated for $t = t_0 = 0$, yield the unit matrix:

$$\begin{aligned} \hat{\Phi}_{11}(t) &= e^{\alpha t}\cos(\sin t) \qquad & \hat{\Phi}_{12}(t) &= e^{\alpha t}\sin(\sin t) \\ \hat{\Phi}_{21}(t) &= -e^{\alpha t}\sin(\sin t) \qquad & \hat{\Phi}_{22}(t) &= e^{\alpha t}\cos(\sin t) \end{aligned} \qquad \text{(A-22)}$$

We can also solve (A-21) by defining the new functions $x_1'(t)$ and $x_2'(t)$ by,

$$x_1 = x_1' e^{\alpha t} \ , \quad x_2 = x_2' e^{\alpha t}$$

(A-21) now becomes

$$\dot{x}_1' = x_2' \cos t \ , \quad \dot{x}_2' = -x_1' \cos t \ ,$$

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* Kamke, Vol. I, p. 611.

or

$$dx_1'/d(\sin t) = x_2' , \quad dx_2'/d(\sin t) = -x_1'$$

so that

$$d^2x_1'/d(\sin t)^2 + x_1' = 0 .$$

This second order equation may be solved by elementary methods to recover the solutions obtained by Kamke's prescription.

The indices on the $\hat{\phi}$'s which appear in (A-22) have again been chosen so that $\hat{\phi}_{ij}(t)$ is the i-th function in the j-th set of solutions. Since $P = 2\pi$, (A-12) for this particular example becomes:

$$\det \begin{vmatrix} \exp(2\pi\alpha) - s & 0 \\ 0 & \exp(2\pi\alpha) - s \end{vmatrix} = 0$$

s is obviously doubly degenerate and equal to $\exp(2\pi\alpha)$. Associated with s are the following two linearly independent eigenvectors: (1,0) and (0,1) . The Floquet Normal Modes, then, are just the solutions given in (A-22) and therefore the Floquet Normal Modes form a fundamental set of solutions to equations (A-21). In addition, for this simple example, we can make the following identifications:

$\mu = i\alpha$; $y_{11}(t) = y_{22}(t) = \cos(\sin t)$; $-y_{21}(t) = y_{12}(t) = \sin(\sin t)$

$$\text{and} \quad \tilde{x}_{ij}(t) = e^{\alpha t} y_{ij}(t) \qquad i,j = 1,2 \ .$$

With the example concluded, we can now proceed to "case (b-2)," i.e., the matrix in (A-12) has a doubly degenerate eigenvalue and this eigenvalue has one and only one linearly independent eigenvector associated with it. The theorem which applies in this case is Theorem IV and from it we obtain the "Form III" solutions which are given by equations (III-10) and (III-11) in the main body of the report. <u>Theorem IV: If (A-12) has only (n - 1) distinct roots because the (n - 1)-th root is doubly degenerate and if there exists one and only one linearly independent eigenvector associated with this doubly degenerate root s_{n-1}, then there are (n - 1) solutions of the form</u>

$$\{\tilde{x}_{ik}(t) = e^{-i\mu_k t} y_{ik}(t)\} \qquad \begin{array}{l} i = 1, \ldots, n \\ k = 1, \ldots, n-1 \ . \end{array} \qquad \text{(A-23)}$$

<u>and, there is one additional solution of the form</u>

$$\{\tilde{x}_{in}(t) = e^{-i\mu_{n-1} t}[y_{in}(t) + t y_{i,n-1}(t)]\} \quad i = 1, \ldots, n \ . \qquad \text{(A-24)}$$

The μ's are constants there is a total of (n - 1) distinct μ's not differing by $\frac{2\pi k}{P}$ (k equal to zero or any integer). For all $y_{ik}(t)$'s :

$$y_{ik}(t) = y_{ik}(t + P) \qquad i,k = 1, \ldots, n .$$

It is true that the set of solutions composed of solutions (A-23) together with (A-24) forms a fundamental set of solutions to (A-1).

Proving this theorem is a more difficult task than proving Theorem III. From the arguments given in the proof of Theorem II, we know that the first (n - 1) solutions which are given by (A-23) are indeed solutions and do form (n - 1) linearly independent solutions. To complete the proof of Theorem IV, then, we must show that (A-24) is indeed a particular solution by seeing if

(a) the equations for the $y_{in}(t)$'s are consistent with the presumed periodicity of the $y_{in}(t)$'s , i.e., does $\dot{y}_{in}(t) - \dot{y}_{in}(t + P) = 0$ for all $i = 1, \ldots, n$?

(b) the $x_{in}(t)$'s can be expressed in terms of the $\hat{\phi}_{ij}(t)$'s , i.e., the unit diagonal fundamental set.

We must then show that the n solutions described by (A-23) and (A-24) taken together form a fundamental set of solutions.

The reader should note that whenever the index n is used in the following discussion, it <u>always</u> refers to the dimensionality of the original problem as stated by (A-1). It is <u>never</u> used as a running index. We further always call the solution given by (A-24), the n-th solution.

In what follows, we will presume that the solutions given by (A-23) are known and therefore the C_{ij}'s are known for $i = 1, \ldots, n$ and $j = 1, \ldots, n-1$. Define the $n \times 1$ column vectors, $\underset{\sim}{C}_j$, by:

$$\underset{\sim}{C}_j = \begin{pmatrix} C_{1j} \\ C_{2j} \\ \vdots \\ C_{nj} \end{pmatrix} \qquad j = 1, \ldots, n-1 .$$

From the arguments used in the discussion of Theorem II, it is known that these vectors, $\underset{\sim}{C}_j$ $(j = 1, \ldots, n-1)$, form a set of $n - 1$ linearly independent vectors.

In proving Theorem IV, the first thing we will ask is: is the periodicity condition

$$\dot{y}_{in}(t) - \dot{y}_{in}(t + P) = 0 \qquad i = 1, \ldots, n \qquad \text{(A-25)}$$

fulfilled? The answer is "yes". To show this, start off by substituting the particular solution (A-24) into (A-1) in order to obtain:

$$\dot{y}_{in}(t) = i\mu_{n-1}[y_{in}(t) + ty_{i,n-1}(t)] - y_{i,n-1}(t)$$
$$- t\dot{y}_{i,n-1}(t) + \sum_{j=1}^{n} \theta_{ij}(t)[y_{in}(t) + ty_{i,n-1}(t)]$$
$$i = 1, \ldots, n . \qquad \text{(A-26)}$$

Evaluating (A-25) through use of (A-26), and, using the relationships

$$\theta_{ij}(t + P) = \theta_{ij}(t) \; ; \; y_{i,n-1}(t) = y_{i,n-1}(t + P) \qquad i,j = 1, \ldots, n$$

we obtain:

$$\dot{y}_{in}(t) - \dot{y}_{in}(t + P) = P\left[\dot{y}_{i,n-1}(t) - i\mu_{n-1}y_{i,n-1}(t) - \sum_{j=1}^{n} \theta_{ij}(t)y_{i,n-1}(t)\right] . \tag{A-27}$$

$$i = 1, \ldots, n .$$

But, because of the differential equation satisfied by the $y_{i,n-1}(t)$'s (see (A-5)), the term on the right-hand side of (A-27) which is in brackets vanishes. Thus, condition (A-25) is fulfilled.

We must now find out whether or not the particular solution given by (A-24) can be expressed in terms of the unit diagonal fundamental set we called the $\hat{\phi}_{ij}$'s . This is equivalent to finding out whether there exists a set of constants, C_{in} , such that

$$\tilde{x}_{in}(t) = \sum_{j=1}^{n} C_{jn}\hat{\phi}_{ij}(t) = e^{-i\mu_{n-1}t}[y_{in}(t) + ty_{i,n-1}(t)]$$

$$i = 1, \ldots, n . \tag{A-28}$$

From equation (A-28), we get that

$$y_{in}(t) = -ty_{i,n-1}(t) + e^{i\mu_{n-1}t} \sum_{j=1}^{n} C_{jn}\hat{\phi}_{ij}(t)$$

$$i = 1, \ldots, n . \qquad \text{(A-29)}$$

We next impose the condition:

$$y_{in}(t_0 + P) - y_{in}(t_0) = 0 \qquad i = 1, \ldots, n . \qquad \text{(A-30)}$$

By utilizing the fact that $\hat{\phi}_{ij}(t_0) = \delta_{ij}$ and by imposing condition (A-30), we find that the C_{jn}'s must obey the following set of equations:

$$\sum_{j=1}^{n} [\hat{\phi}_{ij}(t_0 + P) - s_{n-1}\delta_{ij}]C_{jn} = Py_{i,n-1}(t_0 + P)e^{-i\mu_{n-1}(t_0+P)}$$

$$i = 1, \ldots, n . \qquad \text{(A-31)}$$

The term on the right-hand side of (A-31) may be related to the $C_{j,n-1}$'s by the following considerations. We know that

$$y_{i,n-1}(t_0 + P)e^{-i\mu_{n-1}(t_0+P)} = \sum_{j=1}^{n} C_{j,n-1}\hat{\phi}_{ij}(t_0 + P)$$

$$i = 1, \ldots, n .$$

But, by hypothesis, the $C_{j,n-1}$'s are such that

$$\sum_{j=1}^{n} C_{j,n-1}[\hat{\phi}_{ij}(t_0 + P) - \delta_{ij}s_{n-1}] = 0 \qquad i = 1, \ldots, n .$$

We therefore have that

$$s_{n-1}C_{i,n-1} = \sum_{j=1}^{n} C_{j,n-1}\hat{\phi}_{ij}(t_0 + P) \qquad i = 1, \ldots, n .$$

We can now rewrite (A-31) in matrix form as:

$$\begin{pmatrix} \hat{\phi}_{11} - s_{n-1} & \hat{\phi}_{12} & \cdots & \hat{\phi}_{1n} \\ \hat{\phi}_{21} & \hat{\phi}_{22} - s_{n-1} & \cdots & \hat{\phi}_{2n} \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \hat{\phi}_{n1} & \hat{\phi}_{n2} & \cdots & \hat{\phi}_{nn} - s_{n-1} \end{pmatrix} \begin{pmatrix} C_{1n} \\ C_{2n} \\ \cdot \\ \cdot \\ C_{nn} \end{pmatrix} = Ps_{n-1} \begin{pmatrix} C_{1,n-1} \\ C_{2,n-2} \\ \cdot \\ \cdot \\ C_{n,n-1} \end{pmatrix} \tag{A-32}$$

In reading (A-32), the reader should take note that the suppressed argument of all the $\hat{\phi}_{ij}$'s is $(t_0 + P)$. (A-32) is a non-homogeneous linear equation for the C_{jn}'s and to see if it has a solution, it is convenient to cast the problem into matrix notation. Define the $n \times n$ matrix $\underset{\approx}{\hat{\phi}}$ by $(\underset{\approx}{\hat{\phi}})_{ij} = \hat{\phi}_{ij}(t_0 + P)$. If the $n \times 1$ column vectors C_j are defined by letting the i-th row of the j-th vector be C_{ij} , then, in matrix form, (A-32) becomes:

$$\hat{\phi} C_n - s_{n-1} C_n = P s_{n-1} C_{n-1} \qquad (A-33)$$

By hypothesis, $\hat{\phi}$ has $n - 2$ non-degenerate eigenvalues and one doubly degenerate eigenvalue and, for such a matrix, there exists a non-singular matrix R such that*

$$R^{-1} \hat{\phi} R = V$$

The matrix V is given by:†

$$V = \begin{pmatrix} s_1 & 0 & \cdot & \cdot & 0 & 0 \\ 0 & s_2 & \cdot & \cdot & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot & s_{n-1} & v \\ 0 & 0 & \cdot & \cdot & 0 & s_{n-1} \end{pmatrix} \qquad (A-34)$$

where v (for our supposed case of there being only one linearly independent eigenvector associated with the root s_{n-1}) is some non-zero number. It is easy to see that V has the same eigenvalues

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* To deduce this result, see Noble, Theorem 11.7 (p. 352) and 11.8 (p. 354).

† In the V matrix all off-diagonal elements are zero except the $((n - 1), n)$-th element which is v.

as $\hat{\Phi}$. It is also easy to see that the eigenvector associated with the eigenvalue s_j $(j = 1, \ldots, n)$ is e_j where e_j is the $n \times 1$ column vector which has all elements zero except the j-th which is unity. In particular we have, that, if I is the $n \times n$ unit matrix

$$(V - s_{n-1}I)e_{n-1} = 0 \qquad \text{(A-35)}$$

and, further, e_{n-1} is the only eigenvector of V associated with the eigenvalue s_{n-1}. Premultiplying (A-33) by R^{-1} (we can do this because R is non-singular), we can write (A-33) as,

$$R^{-1}\hat{\Phi}RR^{-1}C_n - s_{n-1}R^{-1}C_n = Ps_{n-1}R^{-1}C_{n-1} \qquad \text{(A-36)}$$

Because C_{n-1} is an eigenvector of $\hat{\Phi}$ associated with eigenvalue s_{n-1}, we have the following relationships:

$$(\hat{\Phi} - Is_{n-1})C_{n-1} = (\hat{\Phi}R - Rs_{n-1})R^{-1}C_{n-1} = (R^{-1}\hat{\Phi}R - Is_{n-1})R^{-1}C_{n-1}$$

$$= 0 = (V - Is_{n-1})e_{n-1} \qquad \text{(A-37)}$$

We may therefore identify $R^{-1}C_{n-1}$ with e_{n-1} and (A-36) therefore becomes:

$$V(R^{-1} \cdot C_n) - s_{n-1}(R^{-1} \cdot C_n) = Ps_{n-1}e_{n-1} \qquad \text{(A-38)}$$

Showing the explicit structure of (A-38) in (A-39),*

$$\begin{pmatrix} s_1 - s_{n-1} & 0 & \cdot & \cdot & 0 & 0 \\ 0 & s_2 - s_{n-2} & \cdot & \cdot & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot & 0 & v \\ 0 & 0 & \cdot & \cdot & 0 & 0 \end{pmatrix} \begin{pmatrix} (\underset{\approx}{R}^{-1}\cdot \underset{\sim}{C}_n)_1 \\ (\underset{\approx}{R}^{-1}\cdot \underset{\sim}{C}_n)_2 \\ \cdot \\ \cdot \\ (\underset{\approx}{R}^{-1}\cdot \underset{\sim}{C}_n)_{n-1} \\ (\underset{\approx}{R}^{-1}\cdot \underset{\sim}{C}_n)_n \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ Ps_{n-1} \\ 0 \end{pmatrix} \qquad \text{(A-39)}$$

it is easy to see that (A-38) can be solved for $(\underset{\approx}{R}^{-1}\cdot \underset{\sim}{C}_n)$: the $(n - 1)$-th element of $(\underset{\approx}{R}^{-1}\cdot \underset{\sim}{C}_n)$ is arbitrary and the n-th element of $(\underset{\approx}{R}^{-1}\cdot \underset{\sim}{C}_n)$ must be equal to Ps_{n-1}/v . Since P and v are by hypothesis non-zero and since s_{n-1} can never be equal to zero (see arguments in the discussion of Theorem II), $(\underset{\approx}{R}^{-1}\cdot \underset{\sim}{C}_n)_n$ can never be equal to zero. $\underset{\sim}{C}_n$ is recovered from $(\underset{\approx}{R}^{-1}\cdot \underset{\sim}{C}_n)$ by simply premultiplying $(\underset{\approx}{R}^{-1}\cdot \underset{\sim}{C}_n)$ by $\underset{\approx}{R}$. Since a non-singular $n \times n$ matrix multiplying a non-null $n \times 1$ column vector can never yield as a product the null $n \times 1$ column vector, a non-null $\underset{\sim}{C}_n$ exists. Thus we have proved what we set out to prove: Theorem IV is true insofar as there is a particular solution of form (A-24).

We have one simple task left, namely, to prove that the solutions (A-23) together with (A-24) form a fundamental set of solutions to

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* In the $n \times n$ matrix of (A-39) all off-diagonal elements are zero except the $((n - 1), n)$-th element which is v .

(A-1). It is easy to see that $(\underset{\approx}{R}^{-1} \cdot \underset{\sim}{C}_n)$ and $\underset{\sim}{e}_{n-1}$ are linearly independent: i.e., there exists no non-zero scalars, α_1 and α_2, such that

$$\alpha_1 (\underset{\approx}{R}^{-1} \cdot \underset{\sim}{C}_n) + \alpha_2 \, \underset{\sim}{e}_{n-1} = 0$$

From this it follows that there exist no non-zero scalars, α_1 and α_2, such that

$$\underset{\approx}{R}[\alpha_1 (\underset{\approx}{R}^{-1} \cdot \underset{\sim}{C}_n) + \alpha_2 \underset{\sim}{e}_{n-1}] = \alpha_1 \underset{\sim}{C}_n + \alpha_2 \underset{\sim}{C}_{n-1} = 0 \qquad \text{(A-40)}$$

Thus $\underset{\sim}{C}_n$ and $\underset{\sim}{C}_{n-1}$ are linearly independent. Since the set of vectors $\underset{\sim}{C}_1, \underset{\sim}{C}_2, \ldots, \underset{\sim}{C}_{n-1}$ form a linearly independent set and since $\underset{\sim}{C}_n$ and $\underset{\sim}{C}_{n-1}$ are linearly independent, it follows that the set of vectors $\underset{\sim}{C}_1, \underset{\sim}{C}_2, \ldots, \underset{\sim}{C}_n$ form a linearly independent set of vectors. From this fact, the reader can use the arguments already used in Theorems II and III to establish that the set of particular solutions composed of the solutions (A-23) and (A-24) form a fundamental set of solutions to (A-1). For the two-level system, these solutions correspond to what we called "Form III" in part II of the main body of this report.

The proof of Theorem IV being complete, we will conclude this appendix by giving a simple system of differential equations governed by Theorem IV.

Example A3:

Consider a system of differential equations given by (A-41).

$$\dot{x}_1(t) = (\tfrac{1}{2} - \sin t)x_1(t) - \tfrac{1}{2}x_2(t)$$
$$\dot{x}_2(t) = \tfrac{1}{2}x_1(t) - (\tfrac{1}{2} + \sin t)x_2(t) \qquad \text{(A-41)}$$

We can solve (A-41) by first defining x_1' and x_2' through:

$$x_1 = x_1' \exp(\cos t) \ ; \quad x_2 = x_2' \exp(\cos t) \ .$$

(A-41) becomes:

$$\dot{x}_1' = \tfrac{1}{2}(x_1' - x_2') = \dot{x}_2'$$

Since $\dot{x}_1' - \dot{x}_2' = 0$, it must be true that $x_1' - x_2' = k$ where k is an arbitrary constant. From this it follows that the most general solutions for the functions $\{x_1', x_2'\}$ is:

$$x_1' = \frac{kt}{2} + c \ ; \quad x_2' = (c - k) + \frac{kt}{2}$$

We can now recover the most general solution of (A-41) as:

$$x_1 = (\frac{kt}{2} + c)\exp(\cos t) \qquad x_2 = [(c - k) + \frac{kt}{2}]\exp(\cos t) \ .$$

With x_1 and x_2 known, we can let $t_0 = 0$, and find the unit diagonal fundamental set of solutions which are given by:

$$\hat{\phi}_{11}(t) = (2e)^{-1}[t + 2]e^{\cos t} \qquad \hat{\phi}_{12}(t) = -(2e)^{-1}te^{\cos t}$$

$$\hat{\phi}_{21}(t) = (2e)^{-1}te^{\cos t} \qquad \hat{\phi}_{22}(t) = (2e)^{-1}[2 - t]e^{\cos t} \tag{A-42}$$

For these fundamental solutions, the fundamental matrix (Equation (A-12)) with $t_0 = 0$ and $P = 2\pi$ becomes:

$$\det\begin{vmatrix} \pi + 1 - s & -\pi \\ \pi & 1 - \pi - s \end{vmatrix} = 0 \tag{A-43}$$

(A-43) is easily solved for s and we find that $(s - 1)^2 = 0$. Hence, s is doubly degenerate and equal to one. Only one linearly independent eigenvector can be found for $s = 1$ and it is:

$$(1,1) = (C_{11}, C_{21})$$

We therefore have a first particular solution which has the form:

$$\begin{aligned} \tilde{x}_{11}(t) &= C_{11}\hat{\phi}_{11}(t) + C_{21}\hat{\phi}_{12}(t) = (e)^{-1}e^{\cos t} \\ \tilde{x}_{21}(t) &= C_{11}\hat{\phi}_{21}(t) + C_{21}\hat{\phi}_{22}(t) = (e)^{-1}e^{\cos t} \end{aligned} \tag{A-44}$$

(A-44) is a solution of the form given by (A-23). Since $s = e^{-i\mu t}$ we can make the following identifications:

$$\mu = 0 \; ; \quad y_{11}(t) = \frac{1}{e} e^{\cos t} \; ; \quad y_{21}(t) = \frac{1}{e} e^{\cos t}$$

The other Floquet Normal Mode can be found by solving (A-32) written for this example:

$$\begin{pmatrix} \pi & -\pi \\ \pi & -\pi \end{pmatrix} \begin{pmatrix} C_{12} \\ C_{22} \end{pmatrix} = 2\pi \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \text{(A-45)}$$

(A-45) has a solution and it is:

$$C_{12} - C_{22} = 2$$

There is a degree of arbitrariness in (A-46), but we can say that C_{12} and C_{22} can never both be zero. Thus (C_{12}, C_{22}) and (C_{11}, C_{21}) form a linearly independent set of vectors. This is, of course, what is expected on account of our discussion following Theorem IV. For simplicity, choose $(C_{12}, C_{22}) = (2,0)$. Using relationships analogous to those given by (A-44), we obtain the second normal mode:

$$\tilde{x}_{12}(t) = (e)^{-1}[2 + t]e^{\cos t} \; ; \quad \tilde{x}_{22}(t) = (e)^{-1} t e^{\cos t}$$

To put meat on the bare-boned expressions used in Theorem IV, we can make the following identifications:

$$y_{12} = 2e^{-1}e^{\cos t} \; ; \quad y_{22}(t) = 0 \; .$$

To demonstrate that the $\tilde{x}(t)$ solutions form a fundamental set of solutions, form a matrix composed of the $\tilde{x}(t)$ functions, take its determinant and show that the determinant can never vanish. For the simple example at hand,

$$\det\begin{vmatrix} \tilde{x}_{11}(t) & \tilde{x}_{12}(t) \\ \tilde{x}_{21}(t) & \tilde{x}_{22}(t) \end{vmatrix} = -\frac{2}{e^2}\, e^{2\cos t} \neq 0 \quad \text{for all } t \; .$$

Thus, the $\tilde{x}(t)$ functions do indeed form a fundamental set of solutions.

One final word is in order. Because the vector (C_{12}, C_{22}) is non-zero but not unique, the $y_{i2}(t)$ functions can never be both zero, but, they are not unique. They, however, will always be periodic (this follows immediately from Theorem IV).

The Floquet modes may be simply related to the general solution which we have written down immediately preceeding (A-42). To recover the first mode, we merely let $k = 0$ and let $C = (e)^{-1}$. The second Floquet mode may be recovered by letting

$$C = k = \frac{2}{e} \; .$$

APPENDIX B: THE EQUATIONS FOR a*a, b*b AND a*b

In this appendix we derive and briefly discuss the equations for the functions a*a, b*b and a*b .

Define the functions P , Q and R by:

$$P(\tau) = a^*(\tau)a(\tau) \; ; \quad Q(\tau) = b^*(\tau)b(\tau) \; ; \quad R(\tau) = a^*(\tau)b(\tau) \tag{B-1}$$

By differentiating P, Q and R and by using Eqs. (II-4) and (II-5), we find

$$\begin{aligned} \dot{P} &= 2i\alpha\cos\tau[R^*-R] \\ \dot{Q} &= -2\delta Q + 2i\alpha\cos\tau[R-R^*] \\ \dot{R} &= -i(\varepsilon-i\delta + 2\beta\cos\tau)R + 2i\alpha\cos\tau[Q-P] \end{aligned} \tag{B-2}$$

Although Eqs. (B-2) are equivalent to Eqs. (II-4) and (II-5),* they are just as intractable as Eqs. (II-4) and (II-5). When $\delta = 0$, Eqs. (B-2) are, however, related to the easily visualized problem of a constant length magnetic moment vector rotating in space under the influence of a classical magnetic field.

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* Assume P, Q and R are known. The ratio, $b(\tau)/a(\tau)$, is obtained by $[b(\tau)/a(\tau)] = [Q/R]^*$. Knowing $b(\tau)/a(\tau)$, $a(\tau)$ and $b(\tau)$ are found by using Eqs. (VIII-27).

Feynman, Vernon and Hellwarth (1957) have shown that for $\delta = 0$, Eqs. (B-2) are equivalent to the classical vector equation:

$$\frac{d(\underset{\sim}{r}(\tau))}{d\tau} = \underset{\sim}{\omega}(\tau) \times \underset{\sim}{r}(\tau) \qquad \text{(B-3)}$$

If $\underset{\sim}{\omega}(\tau)$ corresponds to a magnetic field and $\underset{\sim}{r}(\tau)$ corresponds to a fixed length magnetic moment vector, the motion of the magnetic moment is found by solving an equation of the form of Eq. (B-3).*

To demonstrate this, let

$$\underset{\sim}{r}(\tau) = (R^*+R)\hat{x} + i(R^*-R)\hat{y} + (P-Q)\hat{z} \qquad \text{(B-4)}$$

$$\underset{\sim}{\omega}(\tau) = 4\alpha\cos\tau\hat{x} - [\varepsilon + 2\beta\cos\tau]\hat{z} \qquad \text{(B-5)}$$

where $\hat{x}$, $\hat{y}$ and $\hat{z}$ are the unit vectors in the x, y and z directions respectively. Simple substitution of Eqs. (B-4) and (B-5) in Eq. (B-3) demonstrates the validity of (B-3). That the vector is a constant length vector is demonstrated by noting that

$$\frac{d}{d\tau}\{(R^*+R)^2 + [i(R^*-R)]^2 + (P-Q)^2\} = 0 .$$

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* See, for example, Goldstein (1965), pp. 176-178. Or see, Pople, Schneider, and Bernstein (1959), Sect. 3-3.

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