CHAPTER IV

DIVERGENCE OF THE PERTURBATION SERIES

" Divergent series are the invention of the devil, and it is shameful to base on them any demonstration whatsoever".

N. H. Abel, 1828.

10. Divergence of the perturbation series

The RSPT (Chapter III) allows one to get an approximation to the eigenvalues (E_n) of a given Hamiltonian operator through a series in powers of a real parameter λ. However, the usefulness of the power series is conditioned by a fundamental question: its convergence.

As we know the computation of the RS coefficients is not a trivial task, but even in case of having them the use of the PT is not straightforward. The second problem to be solved is to sum the perturbation series, when it is divergent or has a finite convergence radius.

The determination of the convergence properties of the RS series makes up a whole chapter in Mathematical Physics and it has received a considerable attention from the beginning of 1970. Such convergence properties are basically determined by the properties of $E_n(\lambda)$ as an analytical function of λ. The singularities of $E_n(\lambda)$ in the λ plane determine the convergence radius of the Taylor series.

$$E_n(\lambda) = \sum_{m=0}^{\infty} E_n^{(m)} \lambda^m \quad . \tag{10.1}$$

Several years ago, Rellich |1,2| and Kato |3,4| gave a sufficient condition for a RS series to have a finite convergence radius. In what follows we show the main results and their applications because a rigorous proof is beyond the interest and level of this work.

The most important result we want to discuss is due to Rellich |1-4|

G. A. Arteca et al., *Large Order Perturbation Theory and Summation Methods in Quantum Mechanics*

and is given in the theorem below:

Theorem 10.1

Let H_0 be a self-adjoint operator and V another linear operator such that $D_V \leq D_{Ho}$. If for every function $\phi \in D_{H_0}$ exist two real positive constants a and b <1 satisfying the condition

$$||V\phi|| \leqq a\ ||\phi|| + b\ ||H_0\phi|| \qquad (10.2)$$

then $H=H_0 + \lambda V$ is a self-adjoint operator $\forall\ \lambda\varepsilon R$ and its eigenvalues $E_n(\lambda)$ and eigenfunctions $\psi_n(\lambda)$ are analytical functions of λ in $\lambda=0$ and can be expanded in power series of λ with non-zero convergence radius.

We now present some examples of systems fulfilling theorem 10.1 for which the PT permits one to obtain convergent expansions for several observables of physical interest.

1) Periodic systems

For the sake of simplicity we consider a plane rigid rotator

$$H_0 = -\frac{d^2}{d\theta^2}\ , \quad 0 \leq \theta \leq 2\pi \qquad (10.3)$$

subjected to a nonsingular perturbation $V(\theta)$. However, the argument below applies to other rotational systems as well.

The eigenfunctions and eigenvalues of H_0 are

$$\phi_n = e^{in\phi} \qquad (10.4a)$$

$$E_n = n^2 \qquad n = 0,1,... \qquad (10.4b)$$

since $|V(\theta)|$ is bounded in $(0,2\pi)$; i.e.

$$|V(\theta)| < V_0 \qquad (10.5)$$

we have

$$||H_0 \psi|| = \langle\psi|H_0^2|\psi\rangle^{\frac{1}{2}} \geqq 0 \tag{10.6}$$

$$||V\psi|| = \langle \psi|V^2|\psi\rangle^{\frac{1}{2}} \leqq V_0 \; ||\psi|| \tag{10.7}$$

from which it follows that the inequality (10.2) is satisfied for all $a>V_0$. It si therefore concluded that the perturbation series for the eigenfunctions and eigenvalues of H will have nonzero convergence radii.

As a particular case we consider

$$H = - \frac{d^2}{d\theta^2} + \lambda\cos\theta \tag{10.8}$$

whose eigenvalues $E_n(\lambda)$ have isolated double points on the complex λ plane. Every one of such singularities is a crossing point of a couple of eigenvalues /5/.

2) Systems with finite boundary conditions

Consider the Schrödinger equation

$$H\psi = E\psi \quad , \quad \psi(\pm x_0) = 0 \tag{10.9}$$

where

$$H = H_0 + \lambda V \quad , \quad H_0 = - \frac{d^2}{dx^2} \quad , \tag{10.10}$$

and $V(x)$ is nonsingular in $[-x_0,x_0]$. The eigenvalues of H_0 are

$$E_n^{(0)} = (n+1)^2 \pi^2 / (2x_0)^2 \quad , n = 0,1,... \tag{10.11}$$

upon arguing as before we have

$$||H_0\psi|| \geqq E_0^{(0)} \; ||\psi|| \tag{10.12}$$

$$||V\psi|| \leqq V_0 \; ||\psi|| \tag{10.13}$$

from which it follows that

$$a||\psi|| + b||H_0\psi|| \geq a||\psi|| + b\ E_0^{(0)}\ ||\psi|| \qquad (10.14)$$

will be larger than $||V\ \psi||$ provided that

$$a + bE_0^{(0)} \geq V_0$$

since a and b can be found that satisfies this last inequality we conclude that the RSPT series has a nonzero convergence radius.

3) Perturbed oscillators

We now consider perturbed oscillators of the form

$$H = H_0 + \lambda V(x) \quad , \quad H_0 = \frac{1}{2}\ (-\ d^2/dx^2 + x^2) \qquad (10.15)$$

If

$$V(x) = x \qquad (10.16)$$

then

$$||V\psi|| = <\psi|\ x^2|\psi>^{\frac{1}{2}} \leq <\psi\ |\ H_0|\psi>^{\frac{1}{2}} \leq <\psi\ |\ H_0^2|\psi>^{\frac{1}{4}} = ||H_0\psi||^{\frac{1}{2}} \qquad (10.17)$$

from which it follows that a and b values can be found so that the inequality (10.2) is satisfied. This conclusion is in whole agreement with the fact that the eigenvalues of H are given by

$$H = (n + \frac{1}{2}) - \frac{\lambda^2}{2} \quad ; \qquad (10.18)$$

i.e.the RSPT series reduces to two terms and has therefore infinite convergence radius.

In order to treat the perturbations

$$V_k(x) = x^{2k} \quad , k = 1,2,... \qquad (10.19)$$

it is convenient to consider the eigenfunctions and eigenvalues of H_0:

$$H_0\phi_n = (n + \frac{1}{2})\ \phi_n \qquad (10.20)$$

when k=1 Eq. (8.7) leads us to

$$||V_1\phi_n|| = [\ \frac{3}{2}(n + 1/2)^2 + 3/8\ ]^{\frac{1}{2}} \tag{10.21}$$

since $||H_0\phi_n|| = (n + 1/2)^2$ and $||\phi_n|| = 1$ one cannot find two constants a and b satisfying (10.2). For this reason Theorem 10.1 does not give us any information in this case. However, a straightforward calculation shows that the eigenvalues of

$$H = H_0 + \lambda x^2 \tag{10.22}$$

are

$$E_n(\lambda) = (n + \frac{1}{2})\ (1 + \lambda 2\ )^{\frac{1}{2}}\ (1+2\lambda)^{1/2} \tag{10.23}$$

which exhibit a branch point at $\lambda=-1/2$. Therefore the RSPT converges for all $|\lambda| < \frac{1}{2}$.

When k>1 the potentials $V_k(x)$ are more singular at finity than $V_1(x)$ and Theorem 10.1 is not satisfied. Besides, the analytic properties of $E_n(\lambda)$ are not so simple as in the case k=1 and will therefore be discussed later on.

There exists a number of systems of great interest in Physical Chemistry which Theorem 10.1 predicts a convergent RS power series. These systems are embodied in the following theorem due to Kato |3,4|:

<u>Theorem 10.2</u>

> According to Theorem 10.1 the RSPT series will have nonzero convergence radius for a partition of the electrostatic Hamiltonian H
>
> $$H = H_0 + \lambda V \tag{10.24}$$
>
> of a molecule, atom or infinite crystal, provided that V has no stronger singularity than that corresponding to the pole of the Coulombic potential.

This Theorem has a paramount importance in Chemistry, so we deem it appropriate to make some comments on it. Let us remark that the theorem assures us that considering the electron repulsions as a perturbation λV, the power series expansion in λ has nonzero convergence radius. This leads us to a known result: the power series in Z^{-1} for the electronic energy of atoms and molecules are convergent for $Z>Z_0$, with Z_0 finite /6/.

For diatomic molecules (we restrict ourselves to this case for the sake of simplicity) it is important to consider the perturbation potential V as depending on a parameter R (i.e. the internuclear distance). In order to make the discussion even simpler we choose Z=1 (i.e. unit nuclear charges) and the potential reads

$$V = \frac{1}{R} - \sum_{i=1}^{N} \left[|\bar{r}_i - \bar{R}| \right]^{-1} \qquad (10.25a)$$

where N is the number of electrons and $\bar{r}_i$ represents the coordinate of the i-th electron measured from a given coordinate origin, usually coincident with the position of one of the nuclei.

Let us now to re-write (10.25a)

$$V = \lambda\{1 - \sum_{i} \left[|1 - \bar{r}_i\lambda| \right]^{-1}\} \qquad (10.25b)$$

where $\lambda=R^{-1}$.

We see that λ appears within the potential itself, so that the hypothesis of Theorems 10.1 and 10.2 are not satisfied. In fact, it is well known that the series expansion in powers of R^{-1} possess zero convergence radius. We will discuss again this point later on.

There are a large number of systems with great physical importance that do not obey the Kato and Rellich theorems and they give rise to perturbation series with null convergence radius, that is to say, Taylor expansions that do not represent the function in any region of the complex plane λ. Finding out reasons of such divergences is one of the main problems in PT.

Ref./7/ is very valuable as a complete review on the subject and its applications before the discovery of the above mentioned reasons. The first exhaustive works on RS perturbations series with zero convergence radius were made independently and from quite different viewpoints by Bender and Wu /8/ and Simon /9/ on the basis of the anharmonic oscillator model:

$$H = p^2 + x^2 + \lambda x^{2k} = -\frac{d^2}{dx^2} + x^2 + \lambda x^{2k} \qquad (10.26)$$

in particular for the quartic anharmonic oscillator (k=2).

As commented before, the model (10.26) has an utmost importance in Physics and Chemistry and especially interesting is the connection between this system and some field theories (see Appendix C). This particular problem originated the early study of the divergences in PT. The relevance of such study in PT is peculiarly noteworthy when one takes into account that usually some approximation method is the only way to obtain information in field theory, since it is impossible to make the calculation of matrix elements required by the VM or any other non-perturbative technique.

The fact that the RSPT gives rise to a power series with zero convergence radius implies two issues:

i) The eigenvalue E_n is not an analytical function in $\lambda=0$;
ii) The RS coefficients satisfy

$$\lim_{n\to\infty} |E_n^{(m+1)}/E_n^{(m)}| = \infty$$

We devote the remaining of this paragraph to discuss briefly the first point, while the second property will be analysed in the next paragraph.

Several authors have tried to give simple and intuitive explanations for the divergence of the RSP series for the eigenvalues of (10.26). Among them, we can mention the analysis made by Hioe et al /10-12/. The argument is as follows: the operator (10.26) in the momentum repesentation reads

$$H = p^2 - \frac{d^2}{dp^2} + \lambda \frac{d^{2k}}{dp^{2k}} \qquad (10.27)$$

In this case, the Schrödinger equation becomes the Navier-Stokes equation for turbulent fluids. Then, the PT generates a power series expansion in λ, where the perturbation is that term with the derivative of highest order.

It is a well-known mathematical result that such expansion is divergent /10-12/. Obviously, this reasoning, although valid, does not explain the nature of the singularities responsible for such behavior.

Another argument used frequently to determine whether the RS expansion has a zero convergence radius is the so-called "change-of-sign-argument" This proposition was originally introduced by Dyson /13/ to explain the divergence of the power series for the electronic charge appearing in Quantum Electrodynamics. Later on, such explanation was critically reexamined by Killingbeck /14/, and then this subject stirred up a significant controversy about its interpretation and justification /15-19/.

In short, the basic idea is as follows: if the power series converges in a disc of radius $|\lambda_0|$ around the origin; then the series converges for positive and negative λ values provided $|\lambda| < |\lambda_0|$. However, when $\lambda<0$ the anharmonic oscillator does not hold any bound state. For this reason the convergence radius must be zero.

The conclusions derived from the change of sign argument should be taken with care /16,18,19/. The precedent argument assumes implicitly that the RSPT should approach something with a physical meaning, such as the energy of a bound state. But this is not necessarily so, and such an assuption has originated an apparent conceptual confusion /16, 18,19/, just recently cleared up. As a general rule, we can assert that the regular perturbations /4/ (i.e. those satisfying Theorems 10.1 and 10.2) converge to bound states, which is the sense usually asigned to the convergence towards physically meaningful quantities. In a similar way, those asymptotyc divergent perturbations (i.e. expansions with zero convergence radius) usually converge to the real part of the poles of the resolvent for the eigenvalue problems, although it is not through a simple term by term addition. Then, the perturbation series for those systems having singularities at $\lambda=0$ have some meaning for positive and negative values of λ. The main difference lies on the fact that in the first case the RSPT converges to a bound state by way of some appropriate method of sum, and in the second case to the real part of the system resonances.

So, we can assert a central conclusion which is of vital relevance in what follows: the RSPT makes up an algorithm to derive a regular or asymptotyc power series, which when summed with a suitable method yields a quantity with a well defined physical meaning.

Let us recall here that the essential issue about the reason of non-analyticity of $E_n(\lambda)$ at $\lambda=0$ is not disclosed at all by the precedent discussion and the criteria presented before have just a certain predictive value with regard to obtaining or not power series with zero convergence radius.

The detailed explanation of the deep reasons of the divergence requires to know the analytic structure of $E_n(\lambda)$ in the plane. Naturally this is not a very simple matter, and it has been carried out thoroughly for a few eigenvalue problems.

The first system analysed was the quartic anharmonic oscillator /8,9/ and we sum up here the most relevant results:

i) The energy $E_n(\lambda)$ has a periodicity of 6π in $\arg(\lambda)$, i.e. when one turns over $\arg(\lambda)$ from 0 to 6π, the real eigenvalues are recovered for $\mathrm{Re}\ \lambda>0$.

ii) For $\arg(\lambda) \simeq \frac{3\pi}{2}$ and $\frac{9\pi}{2}$ (asymptotic phase) there exist complex conjugated branch points linked by an arc-like branch line (see Fig. 4.1.)

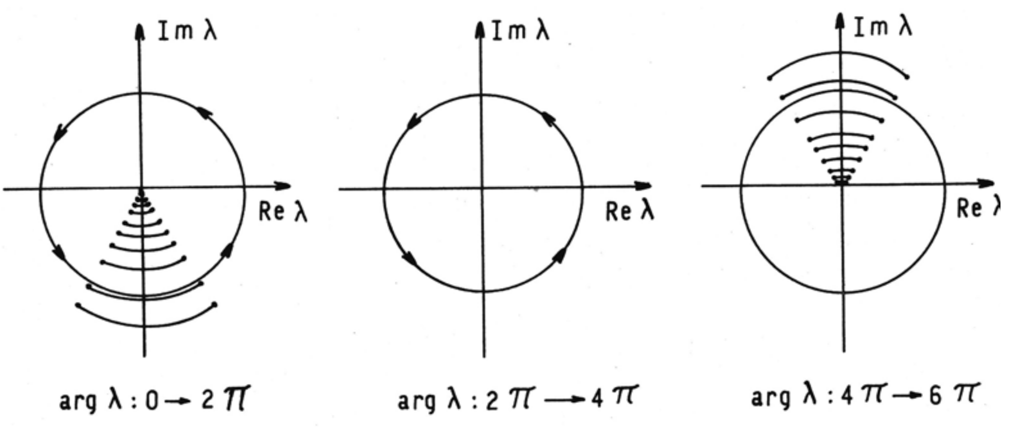

Fig.4.1: Simplified sketch of the $E(\lambda)$ structure (eigenvalue of the quartic anharmonic oscillator) for several sheets of the complex plane λ. Branch point singularities are denoted.

iii) Each pair of branch points (λ_b) corresponds to a crossing point between a pair of eigenvalues as

$$E_n(\lambda_b^{(n)}) = E_{n+1}(\lambda_b^{(n)}) \qquad ; \quad n=0,1,2,... \qquad (10.28)$$

The location of the singularities for the quartic anharmonic oscillator has been calculated by Shanley (P.E. Shanley Phys. Lett. A 117 (1986) 161). The results confirm rigorously some conjectures proposed by Bender and Wu /8/.

These branch points are unique, in the sense that every value only crosses the adjacent one.

iv) The sequence of branch points tends to an accumulation point at the origin $\lambda=0$ (see Fig. 4.1), so that $E_n(\lambda)$ has there a non-isolated singularity. Let us remark that this situation is more complicated than the isolated singularity which gives rise to a finite convergence radius for k=1. (Eq. (10.23)).

All these results remain qualitatively unchanged with respect to the anharmoniticity degree (k=2,3,...) /20/ and the number of terms in the perturbation potential /21/.

Katriel /22/ has proposed a differet alternative to analyse the analytic properties of $E_n(\lambda)$ regarding those viewpoints given by Bender and Wu/8/ and Simon /9/. The discussion presented in this paragraph has intended to give an overview of regular and asymptotyc RSP series and to analyse briefly the reasons of the divergence in a perturbation series.

It remains yet as an open question the way such a divergence reveals itself in the RS coefficients i.e. the rate of divergence of the power series. This poins is examined in detail in the next section.

11. Mathematical Methods to study the Asymptotic Behaviour of the RS coefficients

Let $E(\lambda)$ be an arbitrary function which can be expanded in a Taylor series

$$E(\lambda) = \sum_{n=0}^{\infty} E^{(n)} \lambda^n \qquad (11.1)$$

At the moment we do not make any assuption about the convergence properties of (11.1). Our interest is to compute $E^{(n)}$, $n \gg 1$, for the functions $E(\lambda)$ satisfying some specific properties.

The convergence radius R of (11.1) can be determined from the D'Alembert theorem:

$$\lim_{n\to\infty} |E^{(n+1)}| \; / \; |E^{(n)}| \; = R^{-1} \qquad ; \; R \geq 0 \qquad (11.2a)$$

whenever this limit exists.

Another way to compute R is through the Cauchy-Hadamard theorem:

$$\sup \lim_{n\to\infty} |E^{(n)}|^{1/n} = R^{-1} \qquad (11.2b)$$

where Eq. (11.2b) denotes the superior limit of the sequence of positive numbers $|E^{(1)}|^{\frac{1}{2}}$, $|E^{(2)}|^{\frac{1}{2}}$,... . These theorems make evident the fundamental importance of the asymptotyc behaviour of $E^{(n)}$, $n \gg 1$.

The aim of this section is to determine such behaviour for a wide class of functions, including those with R=0. According to our previous discussion in 10, these functions are of interest in Physics and Chemistry.

In the following we show a very useful relationship, which later on will allow us to compute $E^{(n)}$. Such relationship is the so-called "dispersion relation" and has been presented by several authors /9,23,24/ from quite different viewpoints. Here we introduce an alternative approximation which has some advantages:

Definition I: The power series (11.1) is asymptotic if for every integer m the condition

$$\lim_{|\lambda|\to 0} \{\lambda^{-m}(E(\lambda) - \sum_{i=0}^{m} E^{(i)} \lambda^{i})\} = 0 \qquad (11.3)$$

is satisfied.

In agreement with (11.3), an asymptotic divergent (i.e. R=0) power series possess the following characteristic properties:

i) For a fixed number of terms m, the error diminishes monotonously as λ becomes smaller.

ii) For $|\lambda|<1$ the error diminishes at the beginning as m increases, then remains stationary and finally increases.

The asymptotic series can only give an acceptable approach to $E(\lambda)$ if both $|\lambda|$ and the number of terms in the sum are small enough.

Now let us consider a function $E(\lambda)$ fulfilling the following conditions:

i) $E(\lambda)$ is analytic for $\theta < \pi$, where $\lambda = |\lambda| e^{i\theta}$;

ii) $E(\lambda)$ is asymptotic (Eq. (11.3); and

iii) $$\lim_{|\lambda|\to\infty} E(\lambda) = 0 \qquad (11.4)$$

The discussion below also applies to functions that do not obey (11.4). For instance, if

$$\lim_{|\lambda|\to\infty} |\lambda|^{-\beta} E(\lambda) = e_0 \quad , \quad \beta > 0 \qquad (11.5)$$

we can define a new function

$$E'(\lambda) = \lambda^{-s} \{E(\lambda) - \sum_{n=0}^{s} E^{(n)} \lambda^n\} \quad , \quad \beta < s < \beta + 1 \qquad (11.6)$$

which not only satisfies (11.4) but also gives rise to a power series expansion with the same asymptotic behaviour.

Let λ be a point in the complex plane where E is analytic. Taking the integration path C in the complex plane as shown in figure 4.2

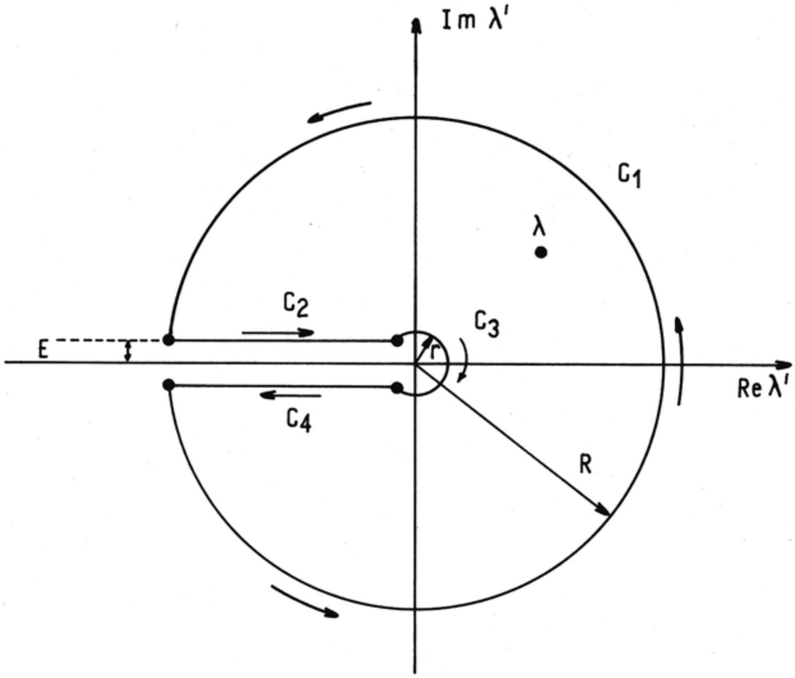

Fig. 4.2: Integration path for E(λ) in the complex plane λ.

the Cauchy theorem assures that

$$E(\lambda) = \frac{1}{2\pi i} \oint_c \frac{E(\lambda')}{\lambda' - \lambda} d\lambda' \quad ; \quad c = \bigcup_{n=1}^{4} c_n \tag{11.7}$$

where c is a Jordan curve. Let us note that c does not cut the negative real axis, where the function is not analytic.

The condition (11.4) leads to

$$\lim_{R \to \infty} \int_{c_1} \frac{E(\lambda')}{\lambda' - \lambda} d\lambda' = 0 \tag{11.8}$$

Furthermore, since

$$\lim_{r\to 0} \int_{C_3} \frac{E(\lambda')}{\lambda' - \lambda} d\lambda' = 0 \qquad (11.9)$$

we have finally that

$$\lim_{\substack{r\to 0\\ R\to\infty}} \oint_C \frac{E(\lambda')}{\lambda' - \lambda} d\lambda' = \lim_{\varepsilon\to 0} \int_{-\infty}^{0} \frac{D(\lambda')}{\lambda' - \lambda} d\lambda' \qquad (11.10a)$$

where

$$D(\lambda') = \frac{1}{2\pi i} \{E(\lambda' + i\varepsilon) - E(\lambda' - i\varepsilon)\} = \frac{\mathrm{Im}E(\lambda' + i\varepsilon)}{\pi} \qquad (11.10b)$$

If (11.10b) is introduced into (11.10a) we find the expression for E(λ) as a generating function for a Stieltjes series /24/

$$E(\lambda) = \frac{1}{\pi} \int_{-\infty}^{0} \frac{\mathrm{Im}E(\lambda')}{\lambda' - \lambda} d\lambda' = \frac{1}{\pi} \int_{0}^{\infty} \frac{\{\mathrm{Im}E(-1/y)/y\}}{1 + \lambda y} dy \qquad (11.11)$$

Upon expanding the integrand of (11.11) in a power series of λ

$$\int_{-\infty}^{0} \frac{\mathrm{Im}\,E(\lambda')}{\lambda' - \lambda} d\lambda' = \int_{-\infty}^{0} \frac{1}{\lambda'} \mathrm{Im}E(\lambda') \left(1 - \frac{\lambda}{\lambda'}\right)^{-1} d\lambda' =$$

$$= \sum_{n=0}^{\infty} \lambda^n \{ \int_{-\infty}^{0} \lambda'^{-n-1} \mathrm{Im}E(\lambda')\, d\lambda' \} \qquad (11.12)$$

and comparing this result with (11.1) we obtain the desired dispersion relation

$$E^{(n)} = \frac{1}{\pi} \int_{-\infty}^{0} \frac{\mathrm{Im}E(\lambda)}{\lambda^{n+1}} d\lambda \qquad (11.13)$$

Eq.(11.13) tells us that the n-th coefficient in the Taylor expansion can be computed fron the knowledge of the imaginary part of E, analytically continued into the complex plane with $|\arg(\lambda)| < \pi$. In other words, the coefficients $E^{(n)}$ are related to the discontinuity of E(λ) through a cut in the Riemann surface.

There are several techniques to obtain the imaginary part of a function E with the above mentioned properties. These procedures have been developed recently and they have provided asymptotic form of the expansion coefficients $E^{(n)}$ (n>> 1) number of models of interest in Physics and Chemistry.

In this section we restrict ourselves to discuss two particular techniques and models of relevance for our present purposes, but they are really representative of the procedures applied to study other systems. In the following we present the results in a detailed manner fo the sake of clearness and to be useful from the pedagogical point of view.

Let us consider the integral (11.14) which is a function whose expansion as a power series in λ has a zero convergence radius:

$$E(\lambda) = \pi^{-\frac{1}{2}} \int_{-\infty}^{+\infty} e^{-(x^2 + \lambda x^4)} dx \qquad (11.14)$$

The integral (11.14) although apparently simple, has not an analytic expression as a function of λ and possess a marked interest in several Physics fields. For example, $E(\lambda)$ represents a zero-dimensional model in Field Theory for a Lagrangian with interaction ϕ^4 /25/, and it has been studied as an elementary test of different approximations /23,26-30/. Besides, (11.14) stands for the classic partition function of a quartic anharmonic oscillator, and so it has been used in Statistical Mechanics /31/. Here, we consider $E(\lambda)$ as an illustrative example, since its simplicity allows one to perform the necessary computation in a closed and rigorous way.

It is quite straightforward to verify that (11.4) is not analytic at the origin because the integral does not exist for $\lambda < 0$. Then, we know that the formal Taylor series for $E(\lambda)$ about $\lambda = 0$ has a null convergence radius.

In order to get some additional information about $E(\lambda)$ we must study its structure as a function depending on a complex variable. This function, the same as those to be studied later on, has two types of singularities:

i) Those due to the multivalued nature of the function which will be termed "trivial" and can be determined through the dilatation relations. They are taken into account in the dispersion relation (11.13) to obtain the asymptotic behavior of the coefficients $E^{(n)}$.

ii) Those singularities called "essential" that determine the analyticity domain of $E(\lambda)$ and which are responsible for the divergence of the power series of λ around $\lambda = 0$.

The first kind of singularity is easily found. In fact, the change of variable $x = \lambda^{-1/4} y$ in Eq.(11.14) gives

$$E(\lambda) = \lambda^{-1/4} \pi^{-1/2} \int_{-\infty}^{+\infty} e^{-(y^4 + \lambda^{-1/2} y^2)} dy \qquad (11.15)$$

The dominant factor $\lambda^{-1/4}$ denotes that the Riemann surface consist of four sheets. That is to say, it is necessary to turn four times around the origin to get the initial value of the function. Consequently, the functions has cuts in the complex plane but it is analytic for $|\arg(\lambda)| < \pi$, as required by Eq.(11.13).

In order to study the analyticity of $E(\lambda)$ in the complex plane, we consider:

$$\lambda = |\lambda| e^{i\theta} \quad ; \quad |\lambda| > 0 \qquad (11.16a)$$

$$x = |x| e^{i\alpha} \quad ; \quad |x| > 0 \qquad (11.16b)$$

The substitutions (11.16a) and (11.16b) into $x^2 + \lambda x^4$ gives

$$x^2 + \lambda x^4 = |x|^2 e^{2i\alpha} + |\lambda| \; |x|^4 e^{4i\alpha + \theta i} \qquad (11.16c)$$

Then, if the integral (11.14) exists(i.e. its real part is finite) the following conditions must be fulfilled:

$$\mathrm{Re}\,\{e^{4i\alpha + \theta i}\} \geqq 0 \qquad (11.17a)$$

$$\mathrm{Re}\,\{e^{2i\alpha}\} \geqq 0 \qquad (11.17b)$$

From (11.17b) it follows that

$$\cos 2\alpha > 0 \;, \text{ then } \; -\pi < 4\alpha < \pi \;. \qquad (11.18a)$$

In a similar way we get from (11.17b) that

$$\cos\,(4\alpha + \theta) > 0 \quad , \text{ then } \quad -\frac{\pi}{2} - 4\alpha < \theta < \frac{\pi}{2} - 4\alpha \tag{11.18b}$$

In order to obtain (11.18) we have restricted ourselves to the first sheet of the Riemann plane. Introducing (11.18a) in (11.18b) we deduce the domain of λ where $E(\lambda)$ is analytic:

$$-\frac{3\pi}{2} < \theta < \frac{3\pi}{2} \quad , \text{ then } \quad |\arg(\lambda)| < \frac{3\pi}{2} \tag{11.19}$$

The last result fixs the domain of λ where there exists a formal λ-power series expansion for $E(\lambda)$.

Nothing has yet been said about the singularities that make $E(\lambda)$ non-analytic in $\lambda=0$. It can be proved that the origin is an accumulative point of branch-point singularities (c.f. the discussion in §.10 for the anharmonic oscillator model).

Let us study some methods to obtain the RS coefficients for $E(\lambda)$. In the present case they can be simply obtained as follows

$$E(\lambda) = \sum_{n=0}^{\infty} E^{(n)} \lambda^n \quad ; \quad E^{(n)} = 2\pi^{-\frac{1}{2}} \frac{(-1)^n}{n!} \int_0^{\infty} x^{4n} e^{-x^2} dx \tag{11.20}$$

Then

$$E^{(n)} = \pi^{-\frac{1}{2}} \frac{(-1)^n}{n!} \Gamma(2n + \tfrac{1}{2}) \tag{11.21a}$$

which according to the Stirling approximation behaves

$$E^{(n)} \cong \pi^{-1} \frac{(-4)^n}{2^{\frac{1}{2}}} (n-1)! \tag{11.21b}$$

when $n >> 1$.

We are interested in calculating $E^{(n)}$, $n>> 1$ approximately by general procedures. In this spirit, we show here two different approximations

Method I: A simple way to compute (11.20) in an approximate manner is by means of the saddle point, or steepest descent method, which is presented in a detailed form in the Appendix D.

Since the integral (11.20) can be written as

$$\int_0^\infty e^{-x^2} x^{4n} dx = \int_0^\infty e^{f(x)} dx \quad ; \quad f(x) = 4n \ln x - x^2 \tag{11.22}$$

it can be approximately computed by finding the largest contribution of the integrand.

We have

$$f'(x_0) = 0 \quad ; \quad x_0 = (2n)^{\frac{1}{2}} \tag{11.23}$$

which is a maximum because

$$f''(x_0) = -4 \tag{11.24}$$

From (11.23) and (11.24) we can expand f(x) around x_0 in a Taylor series up to the second order

$$f(x) = f(x_0) - 2(x - x_0)^2 + \ldots \; ; \; f(x_0) = 2n \ln(2n) - 2n \tag{11.25}$$

and then substitute this result into (11.22) to obtain

$$\begin{aligned} \int_0^\infty e^{f(x)} dx &\simeq e^{f(x_0)} \int_0^\infty e^{-2(x-x_0)} dx = \\ &= e^{f(x_0)} \int_{-x_0}^\infty e^{-2y^2} dy \simeq 2e^{f(x_0)} \int_0^\infty e^{-2y^2} dy \end{aligned} \tag{11.26}$$

In (11.26), we have considered that $x_0 >> 1$. The substitution of (11.25) in (11.26) accomphishes the calculation

$$E^{(n)} \simeq 4\pi^{-\frac{1}{2}} \frac{(-1)^n}{n!} e^{f(x_0)} \int_0^\infty e^{-2y^2} dy - \frac{(-4)^n}{2^{\frac{1}{2}}\pi} (n-1)!$$

This procedure to determine $E^{(n)}$, $n >> 1$, is quite simple and obviously it can only be performed just in some particular cases.

Method II: We apply here the dispersion relation (11.13). Naturally, we must calculate $I_m E(\lambda)$.

The method to be followed is due to Zinn-Justin /23/ and is based on the fact that Eq.(11.13) contains the imaginary part of E along the axis

Re $\lambda<0$ where the function $E(\lambda)$ diverges. Then, we define the parameter

$$\lambda = -g = g\, e^{\pm i\pi} \quad ; \; g > 0 \tag{11.27}$$

and continue x into the complex plane according to (11.16b) so that

$$x^4 = g|x|^4\, e^{4i\alpha \pm i\pi} \tag{11.28}$$

In order to determine $\mathrm{Im}E(\lambda)$ it is necessary to compute $E(\lambda + i.0)$ and $E(\lambda - i.0)$ for $\lambda<0$. To this end we use the definition (11.14) with x-complex. Eq.(11.28) helps us to choose the appropriate paths of integration. In fact, first we set $4i\alpha \pm i\pi=0$ and

$$\alpha_{\pm} = \mp \frac{\pi}{4} \quad ; \; \alpha_{-} = \alpha_{-}(\lambda \to g\, e^{i\pi}); \; \alpha_{+} = \alpha_{+}(\lambda \to g e^{-i\pi}) \tag{11.29}$$

Then, the integration paths are

$$C_{+} : x = |x|\, e^{-i\pi/4} \tag{11.30a}$$

$$C_{-} : x = |x|\, e^{i\pi/4} \tag{11.30b}$$

as shown in Fig.4.3

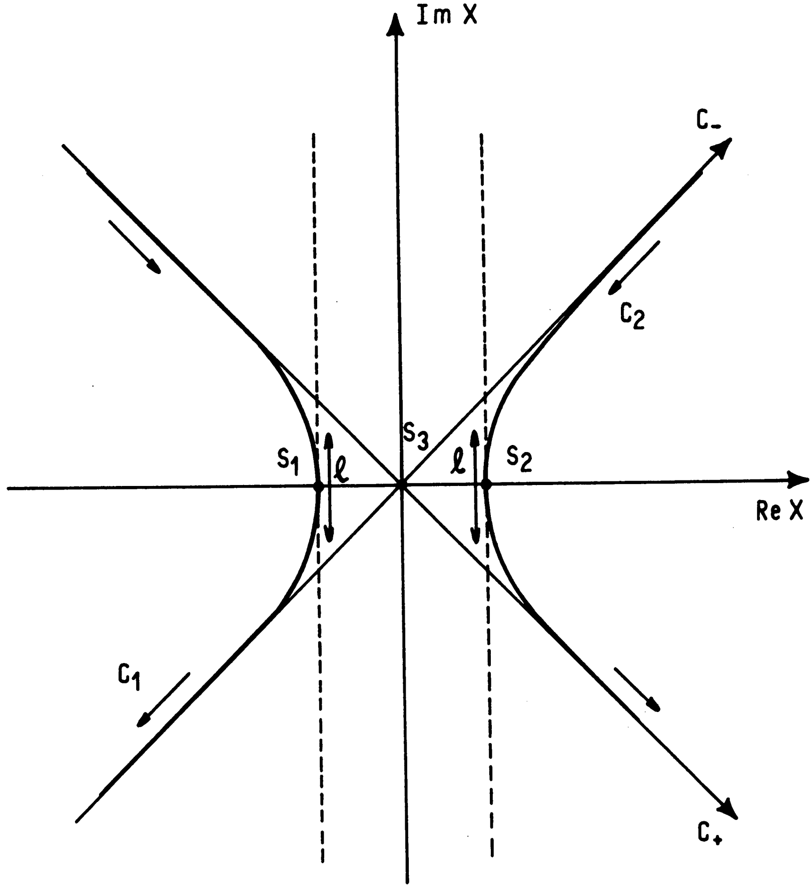

Fig. 4.3: Integration path in the x complex plane to compute ImE(λ) for the integral (11.14).

The notation $c_{\pm}$ denotes the location with respect to the cut in λ (see Fig. 4.2): c_+ and c_- correspond to the second and third quadrants, respectively. Hence,

$$E(\lambda + i.0) = \pi^{-\frac{1}{2}} \int_{c_+} e^{-(x^2 + \lambda x^4)} dx \tag{11.31a}$$

$$E(\lambda - i.0) = \pi^{-\frac{1}{2}} \int_{c_-} e^{-(x^2 + \lambda x^4)} dx \tag{11.31b}$$

Now, we apply the saddle point method to compute the integrals (11.31). The analysis of the function $f(x) = -(x^2 + \lambda x^4)$ allows us to find three stationary points

$$f'(x_0) = 0 \tag{11.32a}$$

$$x_0 : \begin{cases} s_1 = -(-2\lambda)^{-\frac{1}{2}} \\ s_3 = 0 \\ s_2 = (-2\lambda)^{-\frac{1}{2}} \end{cases} \quad , \lambda < 0 \tag{11.32b}$$

with the following second derivatives

$$f''(s_1) = f''(s_2) = 4 \quad , f''(s_3) = -2 \tag{11.33}$$

Then, $f(x)$ has a maximun at the origin and two equidistant minima on the real x axis. On the basis of these results, $f(x)$ can be expanded in a Taylor series around the extrema:

$$f(x) = -x^2 \quad ; \quad x \simeq 0 = s_3 \tag{11.34a}$$

$$f(x) = \frac{1}{4\lambda} + 2(x + (-2\lambda)^{-\frac{1}{2}})^2 \quad ; \quad x \simeq s_1 \tag{11.34b}$$

$$f(x) = \frac{1}{4\lambda} + 2(x - (-2\lambda)^{-\frac{1}{2}})^2 \quad ; \quad x \simeq s_2 \tag{11.34c}$$

Taking into account that from Eq.(11.31) ImE can be written

$$\mathrm{Im}E = \frac{\pi^{-\frac{1}{2}}}{2i} \{ \int_{c_+} e^{-(x^2 + x^4)} dx - \int_{c_-} e^{-(x^2 + x^4)} dx \tag{11.35}$$

then the contribution of s_3 in (11.35) is null when we apply the saddle point method. Therefore, there remains the contribution of s_1 and s_2 (which are different).

In order to compute them it is necessary to distort the integration so that they touch such poits as shown in Fig.4.3. (path C_1 and c_2). Hence, Eq. (11.35) can be rewritten as

$$\mathrm{ImE} = \frac{\pi^{-\frac{1}{2}}}{2i} \{ \int_{c_1} e^{-(x^2 + x^4)} dx + \int_{c_2} e^{-(x^2 + x^4)} dx\} \qquad (11.36)$$

The first integral is computed by means of (11.34b) and it is seen that there is only a significant contribution around s_1, so that (see Fig.4.3):

$$\int_{c_1} e^{f(x)}dx \simeq e^{\frac{1}{4}\lambda} \int_{c_1} e^{2(x + (-2\lambda)^{-\frac{1}{2}})^2} dx \simeq ie^{\frac{1}{4}\lambda} \int_{\ell/2}^{-\ell/2} e^{-2y^2} dy \simeq$$

$$\simeq -i\, e^{\frac{1}{4}\lambda} \int_{-\infty}^{+\infty} e^{-2y^2} dy = -i \left(\frac{\pi}{2}\right)^{\frac{1}{2}} e^{\frac{1}{4}\lambda} \quad , \lambda\uparrow 0 \qquad (11.37)$$

In a similar way we have

$$\int_{c_2} e^{f(x)} dx \simeq -i \left(\frac{\pi}{2}\right)^{\frac{1}{2}} e^{\frac{1}{4}\lambda} \qquad (11.38)$$

and finally we get the desired result (Eq.(11.36)):

$$\mathrm{ImE}(\lambda) = -2^{\frac{1}{2}} e^{\frac{1}{4}\lambda} \quad ; \quad \lambda\uparrow 0 \qquad (11.39)$$

Since the largest contribution to the integral (11.13) comes from $\lambda \simeq 0$, we can obtain the desired result by introducing (11.39) into (11.13):

$$E^{(n)} = \frac{1}{\pi} \int_{-\infty}^{0} \frac{\mathrm{ImE}(\lambda)}{\lambda^{n+1}} d\lambda = - \frac{2^{-\frac{1}{2}}}{} \int_{-\infty}^{0} \frac{e^{\frac{1}{4}\lambda}}{\lambda^{n+1}} d\lambda =$$

$$= \frac{(-1)^n}{2^{\frac{1}{2}}\pi} \int_0^{\infty} y^{n-1} e^{-y/4} dy = \frac{(-4)^n}{2^{\frac{1}{2}}\pi} (n-1)! \qquad (11.40)$$

This result coincides with (11.21) and the computation is made with the help of Method I. The procedure described thus far is basically one of the most frequently employed up to now in order to study the asymptotic behavior of the perturbation coefficients when $n>>1$. The method reveals the close connection between the asymptotic behavior and the discontinuity of the function on the real negative axis of the λ plane. When applying the procedure to other problems, the main difficulty to overcome is to determine ImE. the Method II described above can be generalized to analyse other systems particularly interesting in field theory and quantum mechanics /32-35/. Brizin et al. applied it to different physical quantities within the context of the path integral /36/ and Zinn-Justin discussed the anharmonic oscillator model /23/.

The generalization made by these authors has been quite fruitful and exciting in several respects but it is not the only one. The first approximation to calculate the asymptotic behavior of $E^{(n)}$ has been due to Bender and Wu /8/ via semiclassical methods. From a different, more rigorous point of view, it was proved that Bender and Wu's results are totally correct /9/. The JWKB is certainly simpler than those procedures based on the path integral but it only applies to quantum-mechanical problems. We devote the remain of this paragraph to illustrate in detail the application of the JWKB to the study of the divergence of the RSPT for some anharmonic oscillators.

First of all, we need the following result:

Lemma 11.1 Let us consider the stationary 1D Schrödinger equation

$$-\Psi'' + V(x)\Psi = E\Psi \tag{11.41}$$

Defining the quantum current density J(x) as /37/

$$J(x) = \frac{1}{2i}\{ \Psi \Psi'^* - \Psi^*\Psi' \} = \mathrm{Im}\Psi \Psi'^* \tag{11.42}$$

we have

$$\mathrm{Im}E = J(x) \Big/ \int_{-\infty}^{x} |\Psi(x)|^2 dx' \tag{11.43}$$

Proof:

It is immediate from the consideration of Eq.(11.41) that

$$\Psi^* \Psi'' = (V - E) |\Psi|^2 \tag{11.44a}$$

$$\Psi \Psi''^* = (V - E^*) |\Psi|^2 \quad ; \; V = V^* \tag{11.44b}$$

and so

$$\Psi \Psi''^* - \Psi^* \Psi'' = \frac{d}{dx} (\Psi \Psi'^* - \Psi^* \Psi') = |\Psi|^2 (E - E^*) =$$

$$= 2i \, \mathrm{Im}E \, |\Psi|^2 \qquad (11.45)$$

Finally, the integration of (11.45) gives us the desired result (11.43).

The Lemma 11.1 shifts the problem of determining ImE to the query of obtaining the current density J(x). The determination of J requires studying a problem of penetration through potential barriers, and for this reason we resort to the JWKB method presented in §.6.

Let us consider the anharmonic oscillator

$$H(Z,\lambda) = p^2 + Zx^2 + \lambda x^m \quad ; \; p^2 \quad - \frac{d^2}{dx^2} \qquad (11.46)$$

and let $E(\lambda)$ be one of its eigenvalues. The dispersion relation (11.13) demands the computation of ImE for $\lambda \uparrow 0$, so that, taking into consideration Lemma 11.1, we must determine J for $\lambda \uparrow 0$. If $m > 2$ in (11.46), then for $\lambda > 0$ we have a problem without bound states, there is tunnelling through the barries, and $J \neq 0$. In what follows we consider some illustrative examples.

Example I: If m=3 in (11.43), there are no bound states since the potential is not bounded from below when $x \to -\infty$. Instead there are resonances ε which can be written as

$$\varepsilon = E + \frac{i}{2} \Gamma \qquad (11.47)$$

with E the resonance position and Γ the resonance width. It has been proved that (11.47) is an eigenvalue in some sheet of the complex plane of the Hamiltonian (11.46) analytically scaled /38/. The RSPT provides an asymptotic divergent power series for E (the real part of the resonance)/39/.

To compute $E^{(n)}$ we must have $J(\lambda \uparrow 0)$. The potential function for $\lambda > 0$ is shown in Fig. 4.4

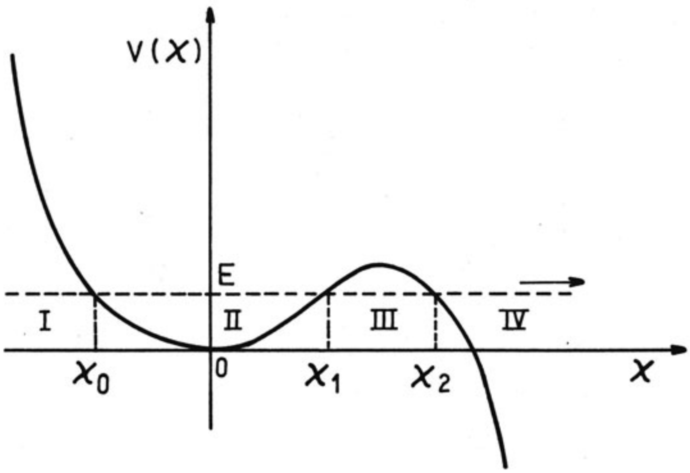

Fig. 4.4: Determination of the RS coefficients asymptotic behavior: resonances problem associated with the cubic anharmonic oscillator.

$$H = p^2 + V \quad ; \quad V = x^2 - gx^3 \qquad ; \; g = -\lambda > 0 \tag{11.48}$$

It is quite clear from Fig. 4.4 that J arises from tunneling towards zone IV. This state of affairs is the same as that discussed in §.6 and shown in Fig. 2.3. According to the results in §.6, J is given by (see Eq.(6.45)):

$$J = \mathrm{Im}\{\Psi_{IV}(x)\, \Psi'^{*}_{IV}\} \quad = -\frac{3}{2\pi} \; |A_2|^2 \tag{11.49}$$

where A_2 is the coefficient for the asymptotic wave function in Zone III (Eq. (6.39)):

$$\Psi_{III}(x) \; \to -e^{i\pi/6} \left(\frac{3}{2\pi q}\right)^{\frac{1}{2}} A_2 \, e^{\tau} \, e^{-|w'|} \tag{11.50}$$

$$\tau = \int_{x_1}^{x_2} (V(x) - E)^{\frac{1}{2}} \, dx \tag{11.51a}$$

$$|w'| = \int_{x_1}^{x} (V(x) - E)^{\frac{1}{2}} \, dx \qquad ; \; x_1 << x << x_2 \tag{11.51b}$$

The classical turning points x_1 and x_2 are shown in Fig. 4.4. To obtain A_2 we proceed as follows: when $\lambda=0$ and $x\to\infty$ the function (11.50) must behave asymptotically as $\Psi_n^{(0)}$, i.e. the zero -order eigenfunction

$$H(\lambda=0)\ \Psi_n^{(0)} = E_n^{(0)}\ \Psi_n^{(0)} \quad ; \quad E_n^{(0)} = 2n + 1 \quad ; \ n=0,1,2,... \qquad (11.52)$$

where n is the number of zeros of the wave function.

In order to obtain the asymptotic behavior of (11.50) as a function of x, we must know τ and w'. To this end we first compute the turning points:

$$x^2 - gx^3 - E = 0 \qquad (11.53)$$

If $g \simeq 0$, then

$$x_0 \simeq -E^{\frac{1}{2}} \quad ; \quad x_1 \simeq E^{\frac{1}{2}} \qquad (11.54a)$$

The third turning point is obtained by considering that $x_2 >> E^{\frac{1}{2}}$ when $g \to 0$:

$$x_2 \simeq 1/g \qquad (11.54b)$$

The integral τ is computed by application of the method proposed in Ref. /38/ , i.e.

$$\tau \simeq \int_{E^{\frac{1}{2}}}^{1/g} (x^2 - gx^3 - E)^{\frac{1}{2}}\, dx = \tau_1 + \tau_2 \qquad (11.55a)$$

$$\tau_1 = \int_{E^{\frac{1}{2}}}^{R} (x^2 - gx^3 - E)^{\frac{1}{2}}\, dx \qquad (11.55b)$$

$$\tau_2 = \int_{R}^{1/g} (x^2 - gx^3 - E)^{\frac{1}{2}}\, dx \qquad (11.55c)$$

where R satisfies the condition $E^{\frac{1}{2}} << R << 1/g$. When $g \to 0$ we have for the integral (11.55b):

$$\tau_1 \simeq \int_{E^{\frac{1}{2}}}^{R} (x^2 - E)^{\frac{1}{2}}\, dx = \frac{1}{2}\ \{ x(x^2 - E)^{\frac{1}{2}} - E\ \ln(x + (x^2 - E)^{\frac{1}{2}})\} \Big|_{E^{\frac{1}{2}}}^{R} \simeq$$

$$\simeq \frac{1}{2}\ \{R^2 + E\ln\,[\frac{E^{\frac{1}{2}}}{2R}]\} - \frac{E}{4} + \ldots \quad ; \quad R >> E^{\frac{1}{2}} \qquad (11.56)$$

To the purpose of computing (11.55c) it is suitable to re-write the integral as

$$\tau_2 = \int_R^{1/g} x\,(1 - gx)^{1/2}\left[1 - \frac{E}{(1 - gx)\,x^2}\right]^{1/2} dx \qquad (11.57)$$

since $x >> E^{1/2}$, we know that

$$\frac{E}{(1 - gx)\,x^2} << 1 \qquad (11.58)$$

On expanding the integrand of (11.57) up to the first order, we have

$$\tau_2 \simeq \int_R^{1/g} x(1 - gx)^{1/2}\,dx - \frac{E}{2}\int_R^{1/g} \frac{dx}{x\,(1 - gx)^{1/2}} \qquad (11.59)$$

The first integral yields

$$\int_R^{1/g} x(1 - gx)^{1/2}\,dx = \frac{2}{15g^2}\,(2 + 3gR)\,(1 - gR)^{3/2} \simeq$$

$$\simeq \frac{4}{15g^2} - \frac{R^2}{2} + 0(g) \qquad (11.60)$$

In a similar way we have /40/

$$\int_R^{1/g} \frac{dx}{x\,(1 - gx)^{1/2}} = - \ln\left[\frac{1 - (1 - gR)^{1/2}}{1 + (1 - gR)^{1/2}}\right] \simeq - \ln\left(\frac{gR}{4}\right) \qquad (11.61)$$

The integral τ_2 follows from (11.59)-(11.61)

$$\tau_2 = \frac{4}{15g^2} - \frac{R^2}{2} + \frac{E}{2}\ln\,(gR/4) \qquad (11.62)$$

so that

$$\tau \simeq \frac{4}{15g^2} + \frac{E}{2}\ln\left(\frac{gE^{1/2}}{8}\right) - \frac{E}{4} \qquad (11.63)$$

It is worth noticing that the final result does not depend upon R. This fact is hardly surprising since such parameter is arbitrary.

When $g \to 0$ and $E << x << 1/g$, the computation of $|w'|$ yields in Eq. (11.56) up to the same number of terms as

$$|w'| \simeq \int_{E^{1/2}}^{x} (x^2 - E)^{1/2} dx = \frac{1}{2} \{ x^2 (1 - \frac{E}{x^2})^{1/2} -$$

$$- E \ln (x + x (1 - \frac{E}{x^2})^{1/2}) + E \ln E^{1/2} \} \simeq$$

$$\simeq \frac{1}{2} \{x^2 [1 - \frac{E}{2x^2}] - E \ln 2x + \frac{E}{2} \ln E \} =$$

$$= \frac{x^2}{2} - \frac{E}{2} \ln 2x + \frac{E}{4} (\ln E - 1) \qquad (11.64)$$

In order to determine the asymptotic behavior of (11.50) we must study $e^{-|w'|}$ for $x >> E^{1/2}$. Eqs. (11.64) and (11.52) allow us to obtain

$$e^{-|w'|} \simeq (2x)^{E/2} E^{-E/4} e^{E/4} e^{-x^2/2} =$$

$$= 2^{(n + 1/2)} \{[\frac{e}{2n + 1}]^{(n + 1/2)}\}^{1/2} x^{(n + 1/2)} e^{-x^2/2} \qquad (11.65)$$

which holds for all n values.

It seems to be necessary to point out that the result (11.65) does not depend on the anharmonic degree m of the Hamiltonian (11.46), because to obtain (11.65) we have started from (11.64) and the limit condition $g \to 0$. In this last equation there are just those terms corresponding to the harmonic oscillator since only the turning point at $x_I = E^{1/2}$ appears.

Considering that for $x >> x_1$, Eq. (11.51c) reduces to

$$q \simeq x \qquad (11.66)$$

we can easily express the asymptotic behavior ($g \to 0$, $x \to \infty$) of (11.50). In fact, the substitution of Eqs. (11.65) and (11.66) in Eq. (11.50) yields

$$\Psi_{III}(x) \to \{-e^{\tau} \quad A_2 \ e^{i\pi/6} \ (\frac{3}{2\pi})^{\frac{1}{2}} \ [(\frac{2e}{n+\frac{1}{2}})^{(n+\frac{1}{2})}]^{\frac{1}{2}}\}x^n \ e^{-x^2/2} \tag{11.67}$$

Then, it only remains to identify Eq.(11.67) with the asymptotic behavior of $\Psi_n^{(0)}$ (Eq. (11.52)) in order to assure the correct behavior of the semiclassical wave function when $g \to 0$.

The asymptotic behavior of the normalized zero order wave function /37/:

$$\Psi_n^{(0)} = (2^n \ n! \ \pi^{\frac{1}{2}})^{-\frac{1}{2}} \ H_n(x) \ e^{-x^2/2} \tag{11.68a}$$

$$H_n(x) = (-1)^n \ e^{x^2} \ \frac{d^n}{dx^n} \ e^{-x^2} \tag{11.68b}$$

is easily found to be

$$H_n(x) \to (-2)^n \ x^n \tag{11.69a}$$

$$\Psi_n^{(0)} \ (x) \to (-1)^n \ [\frac{2^n}{n! \ \pi^{\frac{1}{2}}}]^{\frac{1}{2}} \ x^n \ e^{-x^2/2} \tag{11.69b}$$

Therefore, it follows from equating (11.69b) and (11.67) that A_2 is given by

$$A_2 = (-1)^{n+1} \ [\frac{2^n}{n!}]^{\frac{1}{2}} \ (\frac{4\pi}{9})^{\frac{1}{4}} \ [\frac{n+\frac{1}{2}}{2e}]^{(2n+1)/4} \ e^{-\tau} \ e^{-i\pi/6} \tag{11.70}$$

and consequently

$$|A_2|^2 = \frac{(2\pi)^{\frac{1}{2}}}{3} \ \frac{1}{n!} \ [\frac{n+\frac{1}{2}}{e}]^{n+\frac{1}{2}} \ e^{-2\tau} \tag{11.71}$$

$$J = -\frac{1}{(2\pi)^{\frac{1}{2}}} \frac{e^{-2\tau}}{n!} \left[\frac{n + \frac{1}{2}}{e}\right]^{(n + \frac{1}{2})} \qquad (11.72)$$

It follows from the discussion above that (11.72) is a general tunnelling expression for any Hamiltonian of the form (11.46) when $\lambda \uparrow 0$.

In order to determine ImE, it is just necessary to consider that

$$\int_{-\infty}^{x} |\Psi|^2 \, dx' \simeq \int_{-\infty}^{+\infty} |\Psi_n^{(0)}|^2 \, dx = 1 \quad , \qquad x >> 1 \qquad (11.73)$$

from which we conclude that Eq.(11.72) represents ImE according with Lemma 11.1.

In particular, using (11.63) we have

$$e^{-2\tau} \simeq \left[\frac{g(2n + 1)^{\frac{1}{2}}}{8}\right]^{-(2n + 1)} e^{n + \frac{1}{2}} \; e^{-8/15g^2} \qquad (11.74)$$

which when introduced into

$$\text{ImE}\,(g) = -\frac{e^{-8/15g^2}}{(2\pi)^{\frac{1}{2}}} \, g^{-(2n + 1)} \, \frac{32^{n + \frac{1}{2}}}{n!} \quad ; \quad g \downarrow 0 \qquad (11.75)$$

Making the appropriate change of variables, it is verified at once that Eq.(11.75) agrees with the result reported by Yaris et al. /38/. Now, we are able to calculate the asymptotic form of the k-th coefficient of the RS perturbation series by way of the dispersion relation (11.13). It is necessary to take into account that since ImE(g) has been computed for $g \downarrow 0$ it is then convenient to re-write (11.13) in terms of $g=-\lambda$, i.e.:

$$E_n^{(k)} = \frac{(-1)^k}{} \int_0^{\infty} \frac{\text{ImE}(g)}{g^{k + 1}} \, dg \qquad (11.76)$$

If (11.75) is introduced into (11.77) we have

$$E_n^{(k)} \simeq - \frac{(-1)^k \, 32^{n+\frac{1}{2}}}{(2\pi^3)^{\frac{1}{2}} \, n!} \int_0^\infty e^{-8y^2/15} \, y^{k+2n} \, dy =$$

$$= \frac{(-1)^{k+1} \, 32^{n+\frac{1}{2}}}{(2\pi^3)^{\frac{1}{2}} \, 2(n!)} \left(\frac{15}{8}\right)^{(k+2n+1)/2} \Gamma\left(\frac{k+2n+1}{2}\right) \tag{11.77}$$

The result for the lowest resonance $n = 0$ is

$$E_n^{(k)} \simeq (-1)^{k+1} \frac{2}{\pi^{3/2}} \left(\frac{15}{8}\right)^{(k+1)/2} \left[\frac{k}{2} - \frac{1}{2}\right]! \tag{11.78}$$

where the following notation is used: $\Gamma(a+1) = a!$.

We deem it meaningful to point out that in order to calculate E(k), it is only necessary to calculate $\mathrm{Im}E(g)$ for $g \downarrow 0$. This contribution is dominant in the integral only if $k \gg 1$, so that our procedure gives us the asymptotic behavior of the coefficients $E_n^{(k)}$ for $k \gg 1$.

Example II: Now we consider the quartic anharmonic oscillator (i.e. $m = 4$ in Eq.(11.46)) which was the first system studied with regard to the asymptotic behavior of the RSPT. Krieger /41/ performed a primary simplified analysis, but the first complete results are due to Bender and Wu /8/ and Simon /9/. Here we apply the procedure followed in Example I, which is practically the same as that used in Ref. /42/. It is necessary to calculate the discontinuity of $E(\lambda)$ through the negative λ axis. In this region the potential function is

$$V(x) = x^2 - gx^4 \quad ; \quad g > 0 \tag{11.79}$$

which is shown in Figure 4.5.

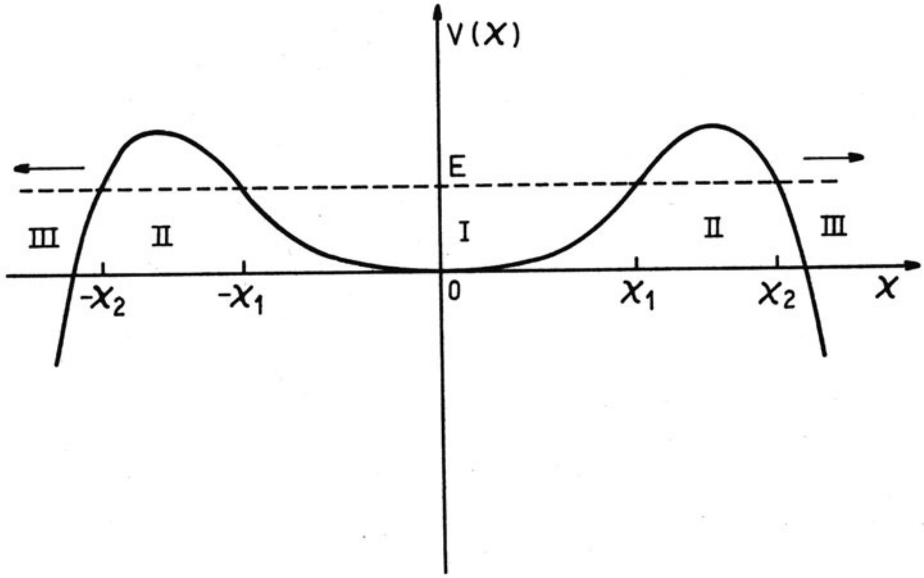

Fig. 4.5: Determination of the RS coefficients asymptotic behavior: resonances problem associated with the quartic anharmonic oscillator.

The potential is even and in this case there is tunneling towards zone IV. Obviusly, the contribution to the probability current density in both zones is the same.

The procedure to be followed is the same as that described in Example I. If J denotes the flux through one of the barriers, then Lemma 11.1 and Eq. (11.73) allow us to write in this case

$$\operatorname{Im} E(\lambda) = 2\, J(\lambda) \tag{11.80}$$

where J is given by (11.72). Evidently, the main difference between both problems rests upon the analytical form of τ.

The classical turning points for $g \downarrow 0$ approximately are

$$x_1 \simeq E^{1/2} \quad ; \quad x_2 \simeq g^{-1/2} \qquad (11.81)$$

as shown in Fig. 4.5. The computation of τ is straightforward and the results are

$$\tau = \tau_1 + \tau_2 \qquad (11.82a)$$

$$\tau_1 = \int_{E^{1/2}}^{R} (x^2 - gx^4 - E)^{1/2}\, dx \qquad (11.82b)$$

$$\tau_2 = \int_{R}^{g^{-1/2}} x(1-gx^2)^{1/2} \left|1 - \frac{E}{x^2(1-gx^2)}\right|^{1/2} dx$$

$$E^{1/2} << R << g^{-1/2} \qquad (11.82c)$$

The result for (11.82b) when $g \downarrow 0$ is given by Eq. (11.56). The second integral is

$$\tau_2 \simeq \int_{R}^{g^{-1/2}} x(1-gx^2)^{1/2}\, dx - \frac{E}{2} \int_{R}^{g^{-1/2}} \frac{dx}{x(1-gx^2)^{1/2}} \qquad (11.83)$$

The two terms in (11.83) can be approximated by

$$\int_{R}^{g^{-1/2}} x(1-gx^2)^{1/2} dx = \frac{1}{3g} (1-gR^2)^{3/2} \simeq \frac{1}{3g} - \frac{R^2}{2} + O(g) \qquad (11.84a)$$

$$\int_{R}^{g^{-1/2}} \frac{dx}{x(1-gx^2)^{1/2}} = \ln \left|\frac{1+(1-gR^2)^{1/2}}{Rg^{1/2}}\right| \simeq \ln \left|\frac{2}{Rg^{1/2}}\right| \qquad (11.84b)$$

Introducing (11.84a) and (11.84b) into (11.83) and adding up (11.56) we have

$$\Gamma \simeq \frac{1}{3g} + \frac{E}{4} \ln \left(\frac{gE}{16}\right) - \frac{E}{4} + \dots \qquad (11.85)$$

The insertion of (11.85) into (11.72) gives for (11.80) the result

$$\mathrm{Im}E(g) = -\left(\frac{2}{\pi}\right)^{\frac{1}{2}} \frac{1}{n!} \left(\frac{8}{g}\right)^{n + \frac{1}{2}} e^{-2/3g} \qquad (11.86)$$

The asymptotic form of the RSPT coefficients in obtained by introducing (11.86) into (11.76), which yields

$$E_n^{(k)} \simeq (-1)^{k+1} \left(\frac{2}{\pi^3}\right)^{\frac{1}{2}} \frac{8^{n+\frac{1}{2}}}{n!} \int_0^\infty y^{k+n-\frac{1}{2}} e^{-2y/3} dy \simeq$$

$$\simeq 2 (-1)^{k+1} \left(\frac{6}{\pi^3}\right)^{\frac{1}{2}} \frac{8^n}{n!} \left(\frac{3}{2}\right)^{k+n} \Gamma(n + k + \tfrac{1}{2}) \qquad (11.87)$$

Once again, after an appropriate change of units we are led to the result published in Refs. /8,42/. Particularly importat for the rest of the book is the analytical asymptotic form of the RS coefficients for the ground state of the quartic anharmonic oscillator (n = 0):

$$E_0^{(k)} \simeq -2 \left(\frac{6}{\pi^3}\right)^{\frac{1}{2}} \left(-\frac{3}{2}\right)^k (k - \tfrac{1}{2})! \qquad (11.88)$$

The analysis presented in this section is especially relevant to understand the properties of the perturbation expansions. Let us remark that in the examples I and II and the function (11.4) analysed previously we have found power series with a zero convergence radius and coefficients increasing approximately as the factorial of the perturbation order. This sort of situation is quite general and the majority of perturbation series arising in eigenvalue problems of interest in Physical Chemistry, field theory, statistical mechanics, etc. have this feature.

It is not our aim to find the asymptotic form of the RS coefficients for mere awkward problems, since the computation is truly complicated. The intention is to present some illustrative examples in order to introduce the large order PT summation methods.

We close this section with the result for the asymptotic coefficients of two problems to be treated later on:

i) Zeeman effect for the hydrogen atom: the perturbation corrections for the ground-state energy of

$$H = -\frac{\Delta}{2} - \frac{1}{r} + \frac{\lambda}{8}\,(x^2 + y^2) \qquad (11.89)$$

behave asymptotically (n >> 1) as /43-45/:

$$E^{(n)} \to (-1)^{n+1}\left(\frac{4}{\pi}\right)^{5/2}\left(\frac{8}{\pi^2}\right)^n (2n + \tfrac{1}{2})\,! \qquad (11.90)$$

ii) Analogously, for

$$H = -\frac{\Delta}{2} - \frac{1}{r} + \lambda r \qquad (11.91)$$

we have /46/

$$E^{(n)} \quad -\frac{18}{\pi e^3}\; n\, n!\; \left(-\frac{3}{2}\right)^n \qquad (11.92)$$

Eqs. (11.90) and (11.92) have been obtained by means of techniques which represent variations or generalizations of the two methods presented in this pharagraph: the contour integral and the JWKB method.

There are other interesting systems having similar behaviors as those discussed here, and they will be analysed afterwards in succeeding chapters of this book.

It is important to point out a feature shared by all the examples presented so far: the k-th coefficient posses the general expression

$$E^{(k)} \sim a\, k^{b}\, c^{k}\, (k!) \tag{11.93}$$

where a, b and c are real numbers.

The knowlwdge of the general form of the RS coefficient for $k >> 1$ has a remarkable importance to tackle the remaining central problem: to extract useful information from the divergent power series, in such a way that one can calculate $E(\lambda)$ for all λ-values.

The study of this fundamental problem(more precisely, the pertúrbation series) is the aim of practically the rest of this book.

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