

**REVIEW AND APPLICATION OF  
THE BENDERWU MATHEMATICA PACKAGE**

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A thesis submitted to the Department of Mathematics and Natural Sciences  
in partial fulfillment of the requirements for the degree of Bachelor of Science  
in Physics

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# Declaration

It is hereby declared that

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3. The thesis does not contain material which has been accepted, or submitted, for any other degree or diploma at a university or other institution.
4. I have acknowledged all main sources of help.

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# Approval

The thesis titled “Review and Application of the BenderWu Mathematica Package” submitted by Tasni Ahsan (14111002) of Summer,2014 has been accepted as satisfactory in partial fulfillment of the requirement for the degree of Bachelor of Science in Physics on 27 December,2018.

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# Abstract

This thesis is the application of the BenderWu Mathematica package to different physical systems. The code was developed to calculate wave function and energy data of higher order perturbation theory in quantum mechanics. The review is done by practical application of the code on the potentials in the examples accompanying the package, as well as the application of it on novel potentials of various forms. The development of the recursion relation behind the code, and the generalization of the relation are also discussed. Finally, the relation between higher order perturbation theory and non-perturbative information encoded in it is also discussed.

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# Chapter 1

## Introduction

The role of computation in physics has always been imperative and is becoming more relevant in recent times, because of its ability to complement both theoretical and experimental works. Initially the need for computers was because of calculations which were too time consuming to be done by humans. It started with numerical analysis methods developed by Newton, Raphson, Euler, Runge, Kutta being implemented in programming. However, now the role of computation has become manifold. Computational works in physics today includes simulation of models, visualization of physical studies, testing hypothesis, interpreting complex data sets, guiding experiments. In experimental physics, virtual simulation can replace expensive experiments. And in theoretical physics, it can be used to obtain numerical results to back up theoretical assumptions, ideas and predictions. One such field that needs this type of computation ability is the field of approximate problem solving, such as perturbation theory in Quantum Mechanics.

Perturbation theory consists of mathematical techniques that are used to solve problems and systems approximately, which do not have exact solutions. It does that by dividing the problem into solvable and perturbative parts. If we want to apply the perturbation method to a system, the complex system we are trying to solve, needs to have a mathematical expression to define it. Then a system which closely resembles the problem at hand is selected. The difference is that the resembling system has exact solution. Next, small corrections or “perturbations” are added to the exact solution. The final solution is expressed in the form of a power series. There are a lot of mathematical descriptions and solutions which are included in perturbation theory. For

example, differential equations used to express wave equation or equation of motion, ground state energy in quantum mechanics. These are all perturbation series. In quantum mechanics, time-independent perturbation theory is as old as quantum mechanics itself. It has roots in wave mechanics as well. For this reason sometimes perturbation theory is also called Rayleigh-Schrodinger perturbation theory. Perturbation series shows interesting behaviour in higher order expansion. Higher orders of the perturbative expansion is intimately related with non-perturbative physics. And this phenomena is called resurgence.

Therefore, there has been many studies regarding higher order perturbation series. The connection between large order perturbative expansion and WKB approximation method was established and studied in detail in works of Carl. M. Bender and Tai Tsun Wu, who studied anharmonic oscillator. They developed recursion techniques to generate very high orders of perturbation theory efficiently and with precision. These analytic techniques are known as Bender-Wu method. Since then this method has been used and applied in variety of studies.

These recursion relations were later generalized by Mithat Unsal and Tin Sulejmanpasic for locally harmonic potentials in quantum mechanics, to determine perturbative wavefunction and energy correction to an arbitrary order. Then the algorithm of this recursion relation was implemented in a Mathematica code. This code is named the BenderWu code and can be used in home computer via the BenderWu Mathematica package, in the Wolfram Mathematica software. This code can be applied on classical, semi-classical and quantum mechanical potentials. The usage and importance of this code is the focus of this thesis.

This thesis is organized as follows: **Chapter-2** looks into the analytic methods introduced by Bender and Wu and the subsequent generalization of those techniques by Sulejmanpasic and Unsal, that went behind the development of the code. **Chapter-3** is a study of the features of the BenderWu code along with its application on a number of potentials of various forms. In **Chapter-4** we implement the code on a potential, which is a part of the derivation of the Hawking radiation as tunneling done by Wilczek and Parikh. **Chapter-5** includes further discussion of the relation of perturbative and non-perturbative physics.

# Chapter 2

## Developing the code

This chapter is dedicated to study the development of the BenderWu Mathematica package and the method, the procedures and the mathematics used behind constructing it. To do that there are two papers which have been studied. One is the paper titled “*Aspects of perturbation theory in Quantum mechanics: The BenderWu Mathematica package*”, authored by the developers of the Package, Tin Sulejmanpasic and Mithat Unsal.

The second paper is “*Anharmonic Oscillator*” written by Carl Bender and Tai Tsun Wu. This paper describes in detail the process of developing the recursion relations, which are known as the Bender-Wu method. Based on this method, later the package was developed by Sulejmanpasic and Unsal.

### 2.1 Adapting the BenderWu method to arbitrary locally harmonic potentials

The paper “*Aspects of perturbation theory*” was written by Tin Sulemanpasic and Mithat Unsal to study perturbation theory in higher order. In this paper a general setup is developed to study the perturbation theory of an arbitrary, locally harmonic 1-D quantum mechanical potential as well as its multivariable generalization.

Time independent perturbation theory is as old as Quantum mechanics itself. It is a center topic in quantum mechanics and was developed by Erwin

Schrodinger. The method is rooted in wave mechanics, and can be dated back to Lord Rayleigh in his book, *The theory of sound*. Although the revelation that large order of perturbation theory has a radius of convergence of zero for most systems, came much later. This is connected to non-perturbative physics. And thus this ties higher order perturbation expansion to non-perturbative theory, making it clear that the perturbative expansion is tied to non-perturbative physics. The study of which falls under Resurgence theory.

In this work the authors adapt the method developed by Carl Bender and Tai Tsun Wu for a perturbative expansion of an arbitrary locally harmonic potential around one harmonic minima. The method was originally for anharmonic oscillator with quartic term in the potential.

The authors also develop a Mathematica code to calculate many orders of perturbation theory.

The code presented here allows a perturbative treatment of one-dimensional systems with a Hamiltonian in the coordinate representation given by:

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial X^2} + V(X) \quad (2.1)$$

Here, the potential  $V(X)$  is a non-singular potential. This potential can be represented as:

$$V(X) = mw^2a^2v(X/a) \quad (2.2)$$

Here,  $v(X/a)$  is a dimensionless function which defines a non-trivial potential.

The paper explains in detail what it defines as a perturbation theory. In the paper the perturbation theory is defined as the expansion of the potential:  $V(X) = mw^2a^2v(X/a)$  around its local minima which coincides with the minima of  $v(X/a)$ . The authors take one such minima and build the perturbation theory around it, still keeping the generality. Thus, in this paper the perturbation series is defined as expansion of the wave-function and energy

in small coupling by the expansion of potential  $v(X/a)$  in powers of  $X/a$ . The non-quadratic terms will be thus treated as perturbations of Harmonic Oscillator.

Treating the non-quadratic terms as perturbation leads to solving the reduced Schrodinger equation for  $\psi(x)$ , the wavefunction and  $\epsilon$  represents the energy as power series.

$$h\psi(x) = \epsilon(x) \tag{2.3}$$

This can be done using the BenderWu method. This method can be generalized for any potential as long as its minima are harmonic and non-singular. Using this method the authors develop recursion relations, which allows the computation of perturbative expansion of wavefunction and energy.

The method is adapted for a potential of the form:

$$V(gx)/g^2 \tag{2.4}$$

This is a general classical potential. The method will also be generalized for some of its quantum effective potentials, such as:

$$V(x) = \frac{1}{g^2}v_0(gx) + v_2(gx) \tag{2.5}$$

and,

$$V(x) = \frac{1}{g^2} \sum_{m=0}^N g^m v_m(xg) \tag{2.6}$$

Any function can be considered to be the potential as long as harmonic minimum is at  $x = 0$ , and is infinitely differentiable at  $x = 0$ .

### 2.1.1 Classical Potential

In the case of the classical 1-D potential  $V(xg)/g^2$ , the Schrodinger equation is:

$$-\frac{1}{2}\psi''(x) + \frac{1}{g^2}v(gx)\psi(x) = \epsilon\psi(x) \quad (2.7)$$

And construct a perturbative expansion around the minimum at  $x = 0$ . The paper then derives the following recursion relations using the BenderWu method:

$$\epsilon_l = -\frac{1}{2}(v+2)(v+1)A_l^{v+2} + \sum_{n=1}^l v_n A_{l-n}^{v-n-2} \quad (2.8)$$

This recursion relation can be now solved for energy  $\epsilon$ .

Here,  $A_l^k$  = coefficient of energy, where rows are related to the index  $l$ , and  $k$  is related to the power of  $x$ . Also,  $v$  = level number of energy.

And the other recursion relation is:

$$A_l^k = \frac{1}{2w(k-v)} \left[ (k+2)(k+1)A_l^{k+2} + 2 \sum_{n=1}^l \epsilon_n A_{l-n}^k - 2 \sum_{n=1}^{l-1} v_n A_{l-n}^{k-n-2} \right] \quad (2.9)$$

Which can be used to solve for the coefficient  $A_l^k$  recursively. And then from that the wavefunction can be derived.

### 2.1.2 Adding quantum effective action

Along with classical potential, the paper also solves quasi-exactly solvable problems, with the potential in equation (1.5). The recursion relations derived



in this case are:

$$\varepsilon_l = -\frac{1}{2}(v+2)(v+1)A_l^{v+2} + \sum_{n=1}^l (v_n^b A_{l-n}^{v-n-2} + v_n^f A_{l-n}^{v-n}) \quad (2.10)$$

$$A_l^k = \frac{1}{2w(k-v)} \left[ (k+2)(k+1)A_l^{k+2} + \sum_{n=1}^l 2\varepsilon_n A_{l-n}^k - \right. \\ \left. 2 \sum_{n=1}^l (v_n^b A_{l-n}^{k-n-2} + v_n^f A_{l-n}^{k-n}) \right] \quad (2.11)$$

This algorithm is the core of the Mathematica package. It is implemented to build the code.

### 2.1.3 Generalization of Recursion relation

Unlike the other recursion relations, the recursion relation in this section is not applied to the Mathematica code. Here recursion relation is generalized to arbitrary effective potential of the form:

$$V(x) = \frac{v_0(xg)}{g^2} + v_2(xg) \quad (2.12)$$

Here,  $v_0$  and  $v_2$  are defined as coefficients of expansion.

The recursion relation becomes:

$$A_l^k = \frac{1}{2w(k-v)} \left[ (k+2)(k+1)A_l^{k+2} + \sum_{n=1}^{\infty} 2\varepsilon_n A_{l-n}^k - 2 \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} v_n^m A_{l-n}^{k-n-2+m} \right] \quad (2.13)$$

### 2.1.4 Symmetries and the form of the perturbation series

The corrections odd in  $g$  of the energy series vanishes. This holds if the potential is symmetric under interchange of  $x \rightarrow -x$  and  $g \rightarrow -g$ , which is called  $g$ -parity.

Although the power series of energy is always in even powers of  $g$ , the wave function can also be normalized to contain only powers  $g^l x^k$ , such that  $(l + k)$  is odd.

### 2.1.5 Multivariable case

This is a generalization to multivariable case. The discussions of this section may have direct application to quantum field theory and in the role of resurgence there.

In principle large-order asymptotic growth can be removed and there can be connection found with IR renormalon singularities and resurgence structure.

There is strong possibility that resurgence structure may be present in quantum field theories as well as in quantum mechanical systems.

The recursion relation in the formalism used here takes geometric form. This formalism might be helpful in the long run in determining the relation between non-perturbative physics and perturbation theory.

## 2.2 Analytic tools used to develop the Bender-Wu method

In this section the Bender-Wu method, based on which the code was developed, is discussed in detail. For this the paper “*Anharmonic Oscillator*”, written by Carl Bender and Tai Tsun Wu is studied. In this paper analytic tools are developed to study singularity structure.

The aim of the paper is to shed light on the fact that for a particular model of anharmonic oscillator the perturbation series for the ground state energy diverges. Bender and Wu developed recursion techniques for efficiently generating very high orders of perturbation theory, and compared these results with higher orders of the WKB approximation.

The model is:

$$\left[ -\frac{d^2}{dx^2} + \frac{1}{4}x^4 + \frac{1}{4}\lambda x^4 \right] \phi(x) = E(\lambda)\phi(x) \quad (2.14)$$

The boundary condition is:

$$\lim_{x \rightarrow \infty} \phi(x) = 0 \quad (2.15)$$

However, a direct inspection of the perturbation series does not give any revelation about the nature of the singularity in the complex  $\lambda$  plane that causes the divergence. And to understand the singularity, analytic method were developed.

And these tools are developed in the following techniques:

1. The authors analytically continue the energy level into the complex  $\lambda$  plane and derive some exact properties of the continuation including the exact condition that gives the location of the singularities in the plane.
2. After deriving the condition, the application of the condition requires the approximation of wave function. The approximation of the wave function is done using a technique based on the zeroth order WKB methods in the complex plane.
3. The results from this is used to determine the singularities in the resolvent  $(z - H)^{-1}$ .
4. Then the results of (1) and (2) are combined to find the approximate location of singularities in the analytic continuation of energy levels.

The motivation behind developing this method was that prior to this work, no techniques had been discovered to shed light on the singularities in the fields with divergent perturbation series. Dyson was the first to discuss divergence of perturbation series in field theory. Jaffe proved the divergence of perturbation series in Green's function in self-interacting boson field theories.

The study of anharmonic oscillator is important in field theory because it is a simple model field theory in one-dimensional space time. The technique developed here to locate singularities in this particular field theory can lead to study of other models with increasing complexity.

The major takeaway from the paper "*Anharmonic Oscillator*" is, the finding that, energy levels of the anharmonic oscillator for a given positive real  $\lambda$  are the positive real values of  $E(\lambda)$  on each of the infinite number of branches of a Riemann surface, with each energy level corresponding to a sheet in the surface.

The paper ventures to answer three questions in the process: Whether the perturbation series is convergent for any  $\lambda$  which is not 0. Does the ground state energy have an isolated singularity at  $\lambda=0$ ? Is the resolvent analytic at  $\lambda=0$ ?

The paper also might be of interest to field theorists because of the unexpected analytic properties observed of the energy levels and resolvent. These properties may help give us an idea of vast underlying complexity of a more realistic field theory.

Along with these are the development of methods to describe actual singularity structure of a particular field theory.

In the following sections, the details of the findings of this paper are presented.

### **2.2.1 Ground state energy of the perturbation series**

Here the properties of perturbation series is investigated in detail.

The perturbation series for the ground state energy in the model in equation (2.14), is defined by  $E(\lambda)$ . It is a power series in the coupling constant  $\lambda$ , which takes the form:

$$E_0(\lambda) = \frac{1}{2}m + \sum_{n=1}^{\infty} mA_n \left[ \lambda/m^3 \right]_n \quad (2.16)$$

Two methods are used to calculate  $A_n$ , which is the coefficient in the energy power series. Both the methods illuminate properties of the perturbation series.

Method-1: Feynman diagram can be used to calculate  $A_n$ , as in field theory in perturbation series ground state energy is the sum of all connected Feynman diagrams.

The perturbation series is finite in every order, though the ground state energy is not an analytic function of  $\lambda^\alpha$  about  $\lambda=0$  for any  $\alpha$ . So, the ground state energy is not analytic at the point where  $\lambda$  is zero.

Method-2: Difference equation is used to calculate  $A_n$ . Here they use the differential equation:

$$\left[ -\frac{d^2}{dx^2} + \frac{1}{4}x^4 + \frac{1}{4}\lambda x^4 \right] \phi(x) = E(\lambda)\phi(x) \quad (2.17)$$

The desired difference equation leads to the relation:

$$A_n = -B_{n,1} \quad (2.18)$$

Where  $B_x(x)$  is the polynomial of  $x$ .

Along with this they determined from computer generated calculation of 75 terms of ground state energy the asymptotic growth is:

$$A_n \sim (-1)^{n+1} \left( \frac{6}{\pi^3} \right)^{1/2} \Gamma\left(n + \frac{1}{2}\right) 3^n \quad (2.19)$$

### 2.2.2 Analytic continuation

The previous section is not able to explain the reason for divergence of perturbation series, which means the singularity structure of  $E_0(\lambda)$  in the complex plane is not known from the two methods in the last section.

The analytic continuation of energy level,  $E(\lambda)$ , which is the eigenvalue of the differential equation, into  $\lambda$  plane helps understand some properties of the continuation.

The exact properties of analytic continuation found are:

1.  $E(\lambda)$  can be continued analytically to all points  $\lambda$  where  $\int \phi^2(x, y) dx$  is not 0.
2. At points where  $E(\lambda)$  is analytic, there is no degeneracy in the energy.
3.  $E_1(\lambda)$  is singular at  $\lambda = \lambda_0$ . Thus level crossing only occurs at singularity points of  $E(\lambda)$ .
4. The singularities of  $E(\lambda)$  are of square root type when  $\lambda$  is not 0.

Also,  $\lambda_0$  is a square root type singularity point of  $E(\lambda)$ . This is associated with the double Riemann sheet, so energy level crossing must take place at every point where  $\lambda_0$  does not equal to zero. After understanding the singularities, the next section works on applying the conditions of singularity to find approximation of wave-function.

### 2.2.3 WKB Solutions

To apply the condition of previous section we must know wave function  $\phi$ . In this section we approximate the wave function using zeroth order WKB method.

Two WKB solutions to the differential equation (1.16), lead to a plot in the complex plane. The sectors in which the general boundary condition applies and the turning points are plotted as well in Figure-2.1 for  $arg \lambda = 0, \pi/2, \pi, 3\pi/2$ .

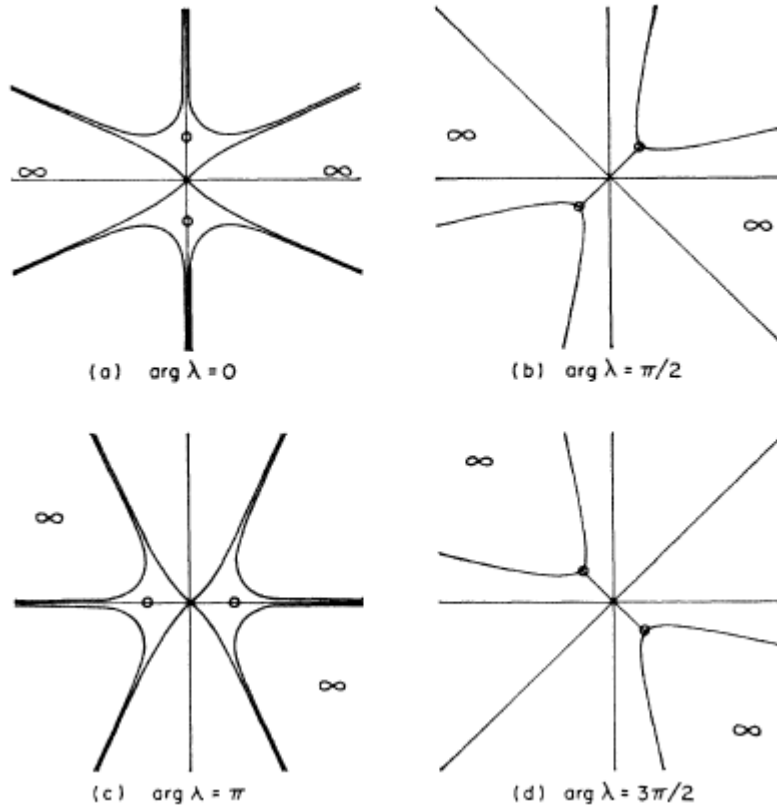


Figure 2.1: Figure:Curves in the complex  $x$  plane.

The figure shows the curves in the complex  $x$  plane where  $Re \lambda^{-1}[(1 + \lambda x^2)^{1/2} - 1] = 0$  for various values of  $arg \lambda$ . The circles denote the turning points and  $\infty$  denotes the sectors.

Through WKB analysis we find four regions: A,B,C and D. WKB procedure is carried out in the four regions and after finding asymptotic behavior of  $\phi$  in all the regions, they are connected across the regions.

$$\frac{\Gamma(\frac{1}{4} + \frac{1}{2}E)}{\Gamma(\frac{1}{4} - \frac{1}{2}E)} = \exp \left[ \frac{i}{3\rho} + \frac{5\pi i}{4} - E \ln \left( \frac{\rho}{2} \right) \right] \quad (2.20)$$

Which is for even parity.

$$\frac{\Gamma(\frac{1}{4} + \frac{1}{2}E)}{\Gamma(\frac{1}{4} - \frac{1}{2}E)} = \exp \left[ \frac{i}{3\rho} - \frac{5\pi i}{4} - E \ln \left( \frac{\rho}{2} \right) \right] \quad (2.21)$$

Which is for odd parity.

These resultant equations may be regarded as approximate equations to zeroth order in  $\lambda$  relating in the low-lying energy levels to complex  $\lambda$  near  $\arg \lambda = 270^\circ$ .

## 2.2.4 Resolvent

Here the location of singularities of the resolvent of the Hamiltonian  $H$  is determined. The authors prove that for both parities the resolvent  $(z - H)^{-1}$  has poles when  $\arg \lambda$  is near  $270^\circ$ .

## 2.2.5 Qualitative Description

In this section the authors discover the properties of the analytic continuation of the energy levels  $E(\lambda)$ , as a function of complex  $\lambda$  in three parts. These parts are as the following:

### Location of branch points

In this section we find the coordinates of branch points of  $E$  in  $\lambda$  plane by solving simultaneously two equations found in equations (1.19) and (1.20) along with this equation:



$$\int \phi^2(x, \lambda) dx = 0 \quad (2.22)$$

After a series of procedures the following equation is found.

$$\frac{1}{\rho} = 6\pi N + 3 - \frac{3\pi}{4} - 3i \left[ \ln(2n)! + \frac{1}{2} \ln\left(\frac{\pi}{2}\right) - \ln(\ln N) - \left(2n + \frac{1}{2}\right) \ln(24\pi N) - 1 \right] \quad (2.23)$$

$$\frac{1}{\rho} = 6\pi N + 3\pi n + \frac{3\pi}{4} - 3i \left[ \ln(2n+1)! + \frac{1}{2} \ln\left(\frac{\pi}{2}\right) - \ln(\ln N) - \left(2n + \frac{3}{2}\right) \ln(24\pi(N+1)) - 1 \right] \quad (2.24)$$

Here,  $\rho$  is a variable introduced for the procedure, defined as,  $\rho = \lambda e^{3\pi i/2}$ . It lists the coordinates of the branch points of  $E(\lambda)$  parametrized by two integers  $N$  (*large*) and  $n$  (*small*).

### Paths on E plane

This section gives a qualitative picture of the complex function  $E(\lambda)$ .

Considering the symmetry properties of  $E$  and considering Hamiltonian is positive definite and Hermitian, the energy levels lie in positive real axis when  $\lambda$  is positive real. Also the energy levels are pure imaginary. The energy levels lie near real axis as  $arg \lambda$  increases from 0 to  $270$ .

The figure-(2.1) gives a picture of  $\lambda$  plane along with the  $E$ -plane.  $\lambda$  plane is shown in three planes, where  $arg \lambda$  ranges from 0 to  $6\pi$ . The brach points and branch cuts are shown schematically.

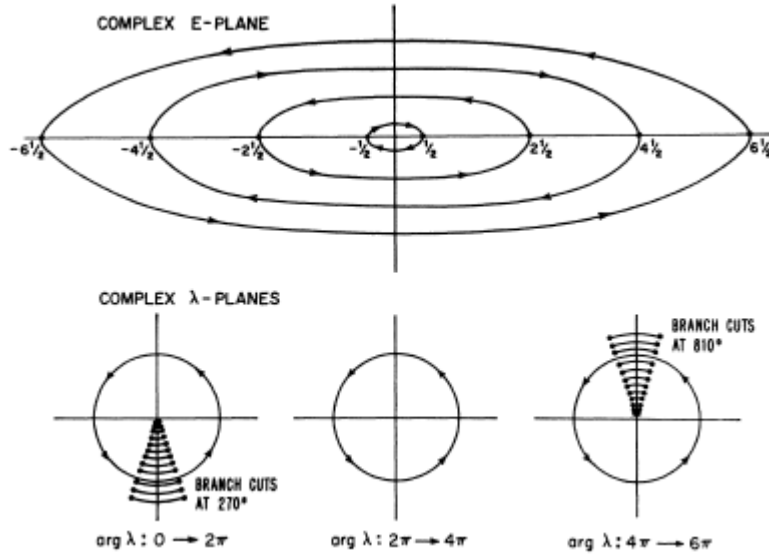


Figure 2.2: A rough picture of the  $\lambda$  plane along with the  $E(\lambda)$  in the  $E$ -plane.

Combining the symmetry properties with these results, predictions can be made.

One prediction is that,  $\lambda$  goes in a circle three times about the origin in the  $\lambda$  plane. Another finding is the branch points do not effect curves in the  $E$ -plane.

Presence of the branch points cannot be detected as long as  $\lambda$  is held fixed.

If the path made by energy level in the complex  $E$ -plane is traced, it can be seen that the energy level returns to positive real axis when  $arg \lambda = 6\pi$ . But it returns to the positive real axis as a different energy level from the original. This is referred to as level crossing.

Thus, it can be said, the physical energy levels for anharmonic oscillator for a given positive real  $\lambda$  are the positive real values of  $E(\lambda)$  on each of the infinite number of branches of a Riemann surface. This is the major result of the paper.

## Level crossing

In the previous section it is mentioned that energy levels in the complex  $\lambda$  plane returns as a different energy level once it crosses branch cuts. This is addressed as level crossing. Which means that energy levels are related to each other by the structure of the branch cuts. That means it is possible to go to one energy level from another different energy level as long as the appropriate branch points are followed.

This section goes into the details of level crossing and gives a pictorial illustration of it through graphs. It is known that level crossing occurs in the  $\lambda$  plane and that it occurs at branch points. In this section, level crossing is investigated in a more detailed manner. The authors try to find which level crossing occur at which point and what does level crossing look like graphically. To answer these questions they conduct intensive numerical calculations. Then they use these calculations to construct graphical representations of level crossings.

The numerical investigation also attempts to answer if the WKB approximation is accurate. And it is found that the numerical results are consistent with the WKB approximations. The results from this part ties in nicely with earlier findings of this paper, such as:

1. At  $\arg \lambda = 180^\circ$ , the WKB turning point enters the sector in which general boundary condition applies. This is just the point where WKB equation is expected to become valid.
2. Bunching phenomena takes place at  $180^\circ$ .
3. The poles of the resolvent occur when  $\arg \lambda$  is larger than  $180^\circ$ .

## Chapter 3

# Description and Application of the BenderWu Mathematica Package

### 3.1 Basic structure of the code

The BenderWu package allows for analytic computation of the perturbation series of a potential in 1-D quantum mechanics around a harmonic minimum of the potential. The code is based on the method pioneered by C. M. Bender and T. T. Wu. The original method was developed by Bender and Wu for anharmonic oscillator with quartic term in the potential.

To execute the code, one must install the Mathematica package in the Wolfram Mathematica, using the package files that can be found in the file accompanying the paper “*Aspects of Perturbation theory in Quantum Mechanics*”. After installing the package, by following the instructions in the file, the package is ready to use. The package is easy to install and contains detailed instructions, examples and tips about running the code. It also is the biggest resource available when it comes to using this code.

The calculation is done by a standard basic syntax. This syntax is different depending on the function one is using.

There are three different functions in the package. They are:

1. The BenderWu function
2. BWProcess function
3. BWLevel polynomials

### 3.1.1 The BenderWu function

The BenderWu function calculates the solution of the differential equation:

$$-\frac{1}{2}\Psi''(x) + \frac{1}{g^2}V_0(gx)\Psi(x) + V_2(gx)\Psi(x) = \Psi(x) \quad (3.1)$$

The function presents the solution as a perturbation series in the coupling of  $g$ :

$$\Psi(x) = \sum_{l,k=1}^{\infty} A_l^k x^k g^l \quad (3.2)$$

$$\epsilon = \sum_{n=1}^{\infty} \epsilon_{2n} \quad (3.3)$$

This function is used to calculate the energy (3.3) and wavefunction data (3.2) of a given potential, up to a given order.

The input consists of four arguments and a number of options. The function is called with the following basic syntax:

BenderWu [ V(x), x, (Level Number), (Order), Options]

In this syntax, there are four arguments and after that a function for calling in various options.

**The first argument:** The first argument is the potential function, which can be input in two basic forms, either by just writing the potential, in which case the entry specifies the classical potential only, or it can be entered as:

```
BenderWu[V0(x), V2(x), x, (LevelNumber), (Order), Options]
```

Here,  $V_0(x)$  and  $V_2(x)$  are the classical and the quantum effective potentials respectively.

**The second argument:** Is the argument of the potential (i.e:  $x$ ). In this argument, the potential which is to be calculated is entered.

**The third argument:** Is the level number at which the potential is being computed.(i.e: The energy level of the potential).

**The fourth argument:** Is the order of  $g^2$ , which is the expansion parameter, to which the energy and wavefunction is computed.

After this there is the arrangement to call for options in the syntax.

### 3.1.2 The BWProcess function

BWProcess function is used to format the output produced by BenderWu function in such a way that is helpful to the user. The user can control the output as he wishes by a number of options provided by the function. The basic syntax:

```
BWProcess[(output Of BenderWu), Options]
```

This function is extremely helpful in making the output data easier to understand. This can be used to output only energy data or only wavefunction

data and that in a preferable form to the user, either in series, matrix or in a graph.

### 3.1.3 The `BWlevelpolynomials` Function

The third function in the package, the `BWLevelPolynomials` computes the perturbative data for multiple values of level number to reconstruct level number dependence. It is useful because the `BenderWu` function does not allow the direct computation of analytic level number dependence.

## 3.2 Implementation of the code

Here, all three functions of the package are reviewed through their application on different potentials. The first five examples were done by the developers of the code in their paper and in the accompanying Mathematica files. The first example is demonstrated in detail in the paper “*Aspects of Perturbation Theory in Quantum Mechanics*”. The second, third, fourth and fifth examples can be found in the Mathematica file accompanying the paper. Following their instructions, these examples were also attempted by us. After that, in the sixth and seventh examples we have applied the code on some other novel potentials, and examined the results in various forms. The potentials in these examples are of higher order polynomial function and trigonometric function.

The takeaway from all these, is that the code can be used to get the energy and wavefunction data in most of these potentials. The calculations are often too big, and that is why it can be a hassle to calculate them in a short time. In that case, one can consider taking advantage of the options available to limit the time spent on calculation, or can ask for the value to be calculated up to a specific order. We used the strategy of not calculating to too high of an order. However, these results are bound to be less illuminating. Also, if the potentials are calculated to a lower order, it will be hard to get the output in the form of a series.

Other than the options built in the functions, there are also other ways to format the output data. When the result is shown, there are a number of

options given to the user in the output box. These give the user more choices in displaying the output. There are options which help in mathematical calculations as well. They can help calculate the transpose of a matrix, factoring of a series, or plotting from the data.

### 3.2.1 Example-1: Computing the energy correction of a potential at a certain level

In this example, the `BenderWu` function is used to compute the first 100 corrections of the perturbation for the third excited state for the potential:

$$\frac{v(xg)}{g^2} = \frac{x^2}{2} + g^2 x^4 \quad (3.4)$$

Here  $g$  is treated as an expansion parameter.

To calculate the data of the potential to the level of 3 and to the order 100, the command is given:

```
In[2] := BW=BenderWu[x^2/2+x^4,x,3,100];
```

After running the code in Mathematica we get an output which needs to be analyzed in terms of three elements. The symbol `BW` is assigned three elements. The first element of the variable `BW` gives a series of corrections. This is the energy series correction. We can get this element by the command:

```
In[4] := BW[[1]]
```

```
Out[4]= [7/2, 75/4, 1575/8, -15184575/128, .....
```

The energy correction is:

$$\epsilon = \frac{7}{2} + \frac{75}{4} + \frac{1575}{8} - \frac{15184575}{128} + \dots$$



The second element, `BW[[2]]` outputs a matrix  $A_l^k$ . Where  $l$  is associated with the power of  $g$  and  $k$  is associated with the power of  $x$ .  $A_l^k$  is the coefficient of the wavefunction. This matrix gives the wavefunction values ( $\psi$ ). The wavefunction can be calculated from  $A_l^k$ , by using :

$$\Psi(x) = \sum_{k,l=1}^{\infty} A_l^k x^k g^l$$

The result is large but it can be presented in a cleaner way using `BWProcess`. When the `BWProcess` function is called it presents the output for the user's suitability.

It returns the eigenvalues:

```
In [5] := BWProcess[BW]
```

```
Out [5] := [7/2, 75/4, 1575/8, -15184575/128, .....]
```

To generate an output which only contains data up to a specific order, one can use the option `Order -> n`, where  $n$  specifies the order (of  $g^2$ ) at which to trim the output, e.g:

```
In [7] := BWProcess[BW, OutputStyle->"Series", Order->2]
```

```
Out [7] = [7/2 + 75g^2/4 - 1575g^4/8 + .....]
```

The energy correction is:

$$\epsilon = \frac{7}{2} + \frac{75g^2}{4} - \frac{1575g^4}{8} + \dots$$

We can also output the wavefunction series,  $u(x)$ , by utilizing the option: `Output -> "WaveFunction"`, in the coupling of  $g$ . This gives:

```
In [8] := BWProcess[BW, OutputStyle->"Series", Order->2,
Output->"WaveFunction"]
```

$$\text{Out [9]} = \frac{3x}{2} + x^3 + g^2 \left( \frac{225x}{16} - \frac{15x^5}{8} - \frac{x^7}{4} \right) + g^4 \left( -\frac{35775x}{128} + \frac{315x^5}{16} + \frac{135x^7}{32} + \frac{115x^9}{192} + \frac{x^{11}}{32} \right)$$

The wavefunction data is:

$$u(x) = \frac{3x}{2} + x^3 + g^2 \left( \frac{225x}{16} - \frac{15x^5}{8} - \frac{x^7}{4} \right) + g^4 \left( -\frac{35775x}{128} + \frac{315x^5}{16} + \frac{135x^7}{32} + \frac{115x^9}{192} + \frac{x^{11}}{32} \right)$$

From running this example it can be said that while the code is quick and easy to use, one must be skilled in interpreting the data output, as it can be hard to analyze.

The large size of the output is also quite difficult to analyze, and it is important to know the usage of the options, to give the output a more manageable look.

### 3.2.2 Example-2: The Double well potential

The examples- 2, 3, 4 and 5 are explained in detail in the Mathematica files accompanying the paper “*Aspects of Perturbation Theory in Quantum Mechanics*”. For all these examples, the classical potential is assumed to be of the form:

$$\frac{1}{g^2} V(gx) \tag{3.5}$$

And the potential has to have a local minimum at  $x = 0$ .

The double well potential will be defined by  $V(x)$ :

$$V(x) = \frac{x^2(x-1)^2}{2} + v_0 \tag{3.6}$$

To execute this code the following syntax is commanded. Here  $V(x)$  is the potential, 3 is the level number of energy and 20 is the order of  $g^2$  to which the data is calculated:

**The Basic syntax:**

`BW = BenderWu[V[x], 3, nu, 20];`

**To calculate the energy data:** If we call the `BenderWu` function to calculate the potential in equation (1.5), without any visualization option, it returns the result in terms of three elements.

The first element would be the energy data. But that result is difficult to decipher. The following are examples of syntax that can be used to call only the energy data, and only in the forms the user desires.

1. To get the output as an array, either of the following syntax will give the same outcome:

```
BWProcess[BW]
```

```
BenderWu[V[x], x, nu, 20, Output -> "Energy"]
```

Which gives the output:

```
Out=[ $-\frac{7}{2}$ , -37,  $\frac{1491}{2}$ ,  $\frac{59093}{2}$ , ...]
```

2. To output the data in series:

```
BWProcess[BW, OutputStyle -> "Series"]
```

3. To output as Matrix:

```
BWProcess[BW, OutputStyle -> "MatrixForm"]
```

4. To change the symbol of expansion parameter:

```
BWProcess[BW, OutputStyle -> "Series", Coupling -> h]
```

5. To truncate the output to a specific order:

```
BWProcess[BW, Order -> 6]
```

6. The BWProcess can be used to plot the energy data as ratio to quickly establish if the series is factorial:

```
ratio = BWProcess[BW, OutputStyle -> "Ratio"];  
ratio // N  
ListPlot[ratio]  
or, to quickly plot:
```

```
BWProcess[BW, OutputStyle -> "RatioPlot"]
```

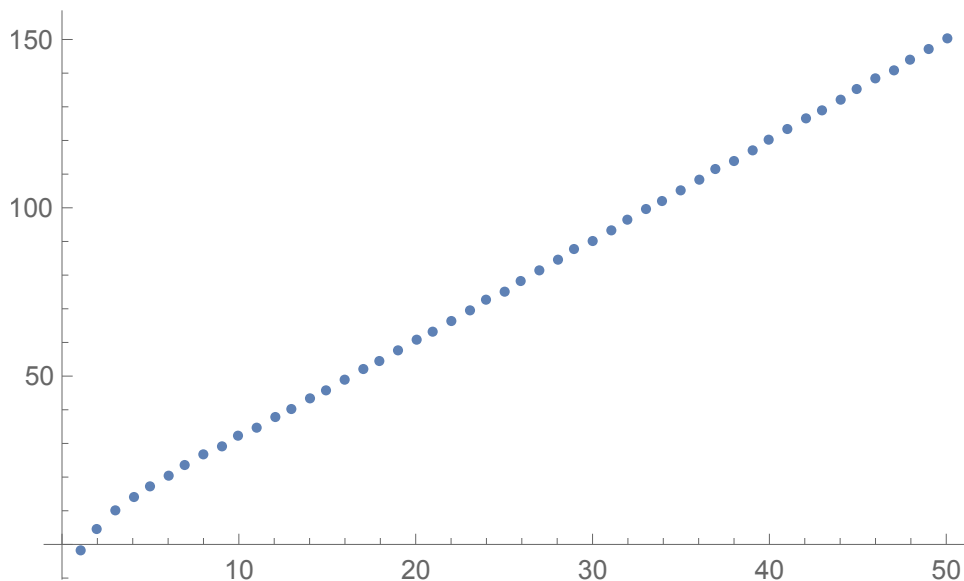


Figure 3.1: Energy Ratio plot

The figure-3.1 shows the result of plotting the energy correction ratio. This plot is used to determine whether the series is factorial.

**To get the Wavefunction Data:** If the function is called without a visualization option, the second element of the output will be used to calculate

the wavefunction using equation (3.2). Other than that, a number of options can be used to present the wavefunction data directly and in desired form.

They are the following:

1. To display only the wave function data, this syntax is used:

```
BWProcess[BW, Output -> "WaveFunction",
OutputStyle -> "Series", Order -> 3]
```

And that gives the result:

$$\text{Out} = [1 + g(x + \frac{x^3}{3}) + \frac{1}{18}g^2x^2(18 + 6x^2 + x^4) + g^3(2x + x^3 + \frac{x^5}{3} + \frac{x^7}{18} + \frac{x^9}{162}) + \dots]$$

2. To change the grouping from of  $x$  to of  $g$ , the following syntax is used:

```
BWProcess[BW, Output -> "WaveFunction",
OutputStyle -> "Series",
Order -> 3,
SeriesOutput -> "Argument"]
```

$$\text{Output} = [1 + (g + 2g^3 + 16g^5)x + (g^2 + \frac{9g^4}{2} + \frac{89g^6}{2})x^2]$$

$$\text{Wavefunction, } u(x) = 1 + (g + 2g^3 + 16g^5)x + (g^2 + \frac{9g^4}{2} + \frac{89g^6}{2})x^2.$$

3. To include pre-exponent, this syntax is used:

```
BWProcess[BW, Output ->
"WaveFunction", OutputStyle -> "Series",
Order -> 3, Prefactor -> True]
```

4. To output the coefficients of the wavefunction as a matrix:

```
BWProcess[BW, Output -> "WaveFunction",
OutputStyle -> "MatrixForm", Order -> 3].
```

### 3.2.3 Example-3: The SUSY double well potential

A Supersymmetric potential of the form:

$$\frac{1}{2}W'(x)^2 + \frac{1}{2}W''(x), \quad (3.7)$$

Can be given the form:

$$\frac{1}{g^2}V(xg) + V_f(xg) \quad (3.8)$$

As, there are two potentials, the first argument of the syntax should be:  $V[x], V_f[x]$ .

The potentials need to be defined in Mathematica first:

```
V[x_] := x^2 (x - 1)^2/2;  
V_f[x_] := (2 x - 1)/2;
```

1. For the ground state energy, the first 50 orders are and for the higher state energy, first 20 orders are calculated respectively by:

```
BenderWu[{V[x], Vf[x]}, x, 0, 50, Output -> "Energy"]
```

```
BenderWu[{V[x], Vf[x]}, x, 3, 20, Output -> "Energy"]
```

For the ground state, energy data is trivial, but for higher states it is trivial and asymptotic.

2. All these calculation can take long amount of time. One can manage this inconvenience by using the options:

```
BenderWu[{V[x], Vf[x]}, x, 3, 50,  
Output -> "Energy", MaxTime -> .02]
```

```
BenderWu[{V[x], Vf[x]}, x, 3, 100,
```

```
Output -> "Energy",
TotalMaxTime -> .005]
```

3. We can use the symbolic parameter  $\zeta$  to get the energy output as its coupling, using:

```
energyzet = BenderWu[Evaluate[{x^2 (x - 1)^2/2, \[Zeta]
(2 x - 1)/2}], x, 0, 10, Output -> "Energy",
Simplify -> True]
```

$\zeta$  here is a parameter and the energy data can be expressed as a coupling in  $\zeta$ , in stead of as a coupling of  $x$  or  $g$ .

Plotting the orders of  $g$  as a function of  $\zeta = 1$  looks like the figure-3.2.

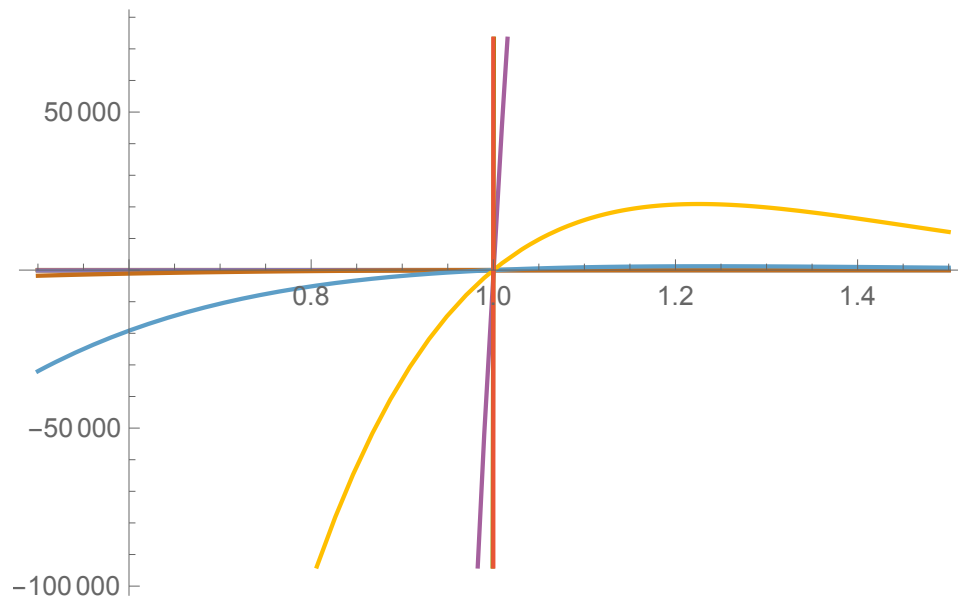


Figure 3.2: Plot of the orders of  $g$  as a function of  $\zeta$ .

The horizontal axis represents the values of  $\zeta$  and the vertical axis shows the orders of  $g$ .

### 3.2.4 Example-4: The Jacobi-Elliptic potential

Jacobi-Elliptic functions are standard forms of elliptic functions. Potentials of this form can be calculated, as the `BenderWu` function can handle any potential as long as it has a polynomial power series around  $x = 0$ . For the Jacobi-Elliptical potential the first argument is: `JacobiSN[x, m]^2`. The syntax to the order of three in the third excited state is:

```
BW = BenderWu[JacobiSN[x, m]^2, x, 3, 10, Simplify -> True];
```

```
BWProcess[BW, Order -> 6]
```

```
Out=[ $\frac{7}{\sqrt{2}}$ ,  $-\frac{25}{8}(m+1)$ ,  $-\frac{7(13-28m+13m^2)}{32\sqrt{2}}$ ,  $-\frac{855}{256}(-1+m)^2(1+m)$ , ...]
```

### 3.2.5 Example-5: Sine-Gordon level dependence of the perturbation theory

If level number is expressed by  $v$ , one can construct the energy data series for each level number from 0 to 6, and that way can establish the level dependence of perturbation theory. To do that, one also needs to use the `BWLevelPolynomial` function to reconstruct the level dependence at each other. Using the syntax:

```
BW3 = Table[BenderWu[Sin[x]^2/2, x, nu, 5,
Output -> "Energy", Monitor -> False], {nu, 0, 7}];
```

```
BW3levels = BWLevelPolynomial[BW3]
```

```
Out=[ $\frac{1}{2} + v$ ,  $-\frac{1}{8} - \frac{v}{4} - \frac{v^2}{4}$ , .....]
```

Thus, the energy correction is:



$$\epsilon = \left(\frac{1}{2} + v\right) + \left(-\frac{1}{8} - \frac{v}{4} - \frac{v^2}{4}\right) + \dots$$

To get the energy series at a specific level:

```
BW3levels[[4]]
```

$$\text{Out} = \left[-\frac{3}{128} - \frac{11v}{128} - \frac{v^2}{8} + \frac{5v^3}{64} + \frac{5v^4}{128}\right]$$

Which is the fourth element, meaning the energy data at the third level.

Energy correction at third level:

$$\epsilon_3 = -\frac{3}{128} - \frac{11v}{128} - \frac{v^2}{8} + \frac{5v^3}{64} + \frac{5v^4}{128}.$$

### 3.2.6 Example-6: Higher Order Polynomial potentials

In this section, there are the results of applying the `BenderWu` functions to a number of Higher Order Polynomial potentials.

1.  $V(x) = x^{10} + x^2 + x^5$ .

The syntax used to output the energy in series of the level number 2:

```
BW = BenderWu[x^10 + x^2 + x^5, x, 2, 5,
Output -> "Energy", OutputStyle -> "Series"];
```

$$\text{Out} = \left[\frac{5}{\sqrt{2}} - \frac{31529g^6}{256} + \frac{57645g^8}{128\sqrt{2}}\right].$$

This output can be displayed in other forms, by utilizing the choices given by Mathematica after the calculation is done. By using the plotting option, we get the plot of the result in Fig-3.3:

In this figure the horizontal axis represents values of  $g$ .

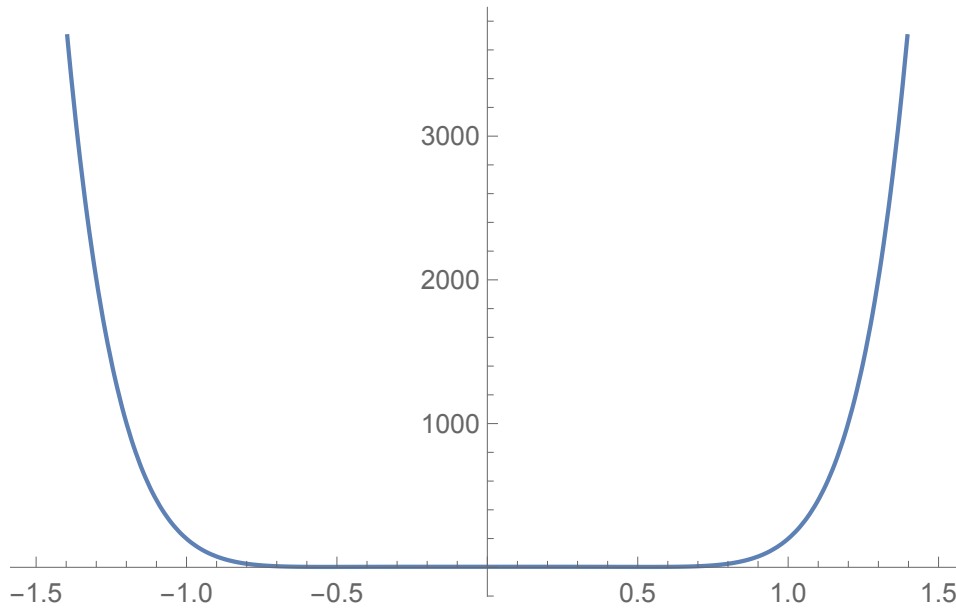


Figure 3.3: Plot of energy series in terms of  $g$

2.  $V(x) = x^8 + \frac{x^2}{2}$ .

For this potential, without using any visualization options, we get the calculation of level number = 2, to the order of 1, by the syntax:

```
BW = BenderWu[x^8 + x^2/2, x, 2, 1];
```

```
Output={0, 5/2, 0}, {{-(1/2), 0, 1, 0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0,
0, 0, 0}}, {x, 2, 2, 1}]
```

Here, first element is the energy data, second element gives wavefunction data.

3.  $V(x) = x^{10} + x^2 + x^5 + x$ .

To get the wavefunction of this potential, this syntax is used:

```
BW = BenderWu[x^10 + x^2 + x^5 + x, x, 2, 1,
```

```
Output -> "Wavefunction",OutputStyle -> "Matrix"];
```

```
Output=[{-(1/2), 0, 0}, {0, 0, 0}, {2, 0, 0},  
{0, 0, 0}, {0, 0, 0}, {0,0, 0}, {0, 0, 0},  
{0, 0, 0}, {0, 0, 0}]
```

4.  $V(x) = x^{21} + \frac{x^2}{2}$ .

For this potential, the syntax used to get the energy data of first 5 orders is:

```
BW = BenderWu[x^21 + x^2/2, x, 2, 5, Output -> "Energy"]
```

```
Output={5/2, 0, 0, 0, 0}
```

```
BW = BenderWu[x^21 + x^2/2, x, 2, 5, Output -> "Energy",  
OutputStyle -> "Series"];
```

```
Output=5/2.
```

### 3.2.7 Example-7: Trigonometric potentials

Potentials which are trigonometric functions can also be calculated by this function. Here are a number of examples which were tried:

1.  $V(x) = \sin\left(\frac{x^2}{2}\right)$ .

The energy was calculated up to order 5 in series form, using the command:

```
BW = BenderWu[Sin[x]^2/2, x, 2, 5, Output -> "Energy",  
OutputStyle -> "Series"];
```

$$\text{Out} = \left[ \frac{5}{2} - \frac{13g^2}{8} - \frac{35g^4}{32} - \frac{249g^6}{128} - \frac{9775g^8}{2048} - \frac{115371g^{10}}{115371g^{10}} \right]$$

Using the application named “Factor”, we get:

Energy series in factorial form:

$$\epsilon = \frac{20480 - 13312g^2 - 8960g^4 - 15936g^6 - 39100g^8 - 115371g^{10}}{8192}$$

And, using the “Plot” application gives the Figure-3.4.

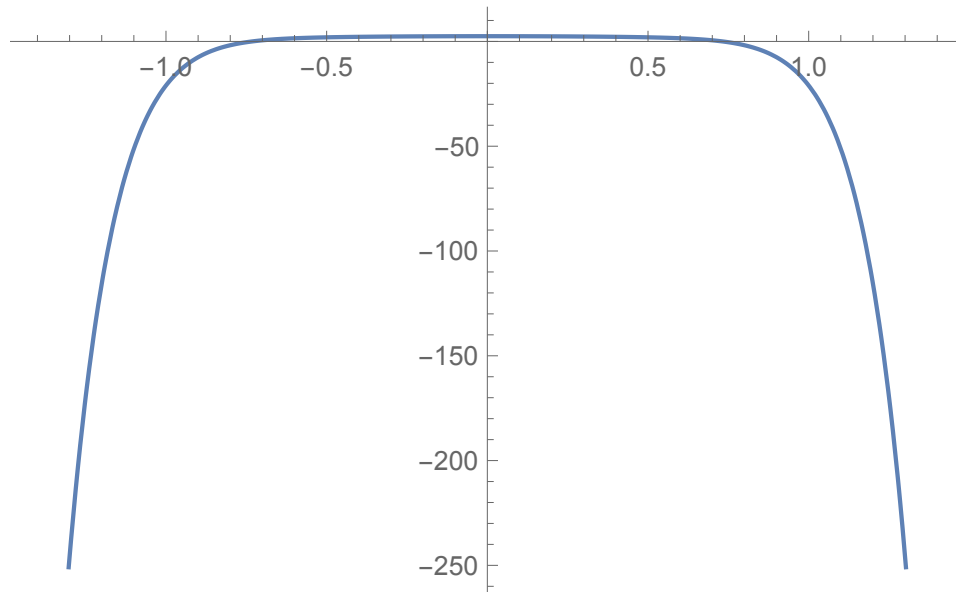


Figure 3.4: Plot of the energy series of the trigonometric function

Here is the plot of the energy series in terms of  $g$ , which is represented in the horizontal axis.

2.  $V(x) = \cos\left(\frac{x^2}{2}\right)$ .

Calculating this potential without any visualization options, gives the energy and wavefunction data:

```
BW = BenderWu[Cos[x]^2/2, x, 2, 1];
```

```
Output={{1/2, (5 i)/2, -(13/8)}, {{-(1/2), 0,
i, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0,
0, 0, 0}, {(13 i)/32, 0, 0, 0, (13 i)/48,
0, -(1/24), 0, 0}}, {x, 2, 2, 1}}
```

3.  $V = \cos x$ .

To get the wavefunction of this potential in a Matrix form, one has to use the syntax:

```
BW = BenderWu[Cos[x], x, 2, 1, Output -> "Wavefunction",
OutputStyle -> "Matrix"];
```

Then use the option “display” in the dialogue box to get the matrix.

### 3.2.8 Example-8: BWDifference function example

The `BWDifference` function computes the perturbative expansion of the eigenvalue problem:

$$h(x, p)\Psi(x) = E\Psi(x) \quad (3.9)$$

Where,  $x = e^g x$  and  $p = e^g p$ , such that the commutator  $[x, p] = i$ . The `BWDifference` function computes an expansion of  $\Psi(x)$  and  $E$  as a power series in  $g$ .

The command is executed by the syntax:

```
BW = BWDifference[X + P + 1/X + 1/P, {X, P}, 2, 10];
```

Which gives the output in terms of three elements.

```
BW[[1]]
```

This gives the first element, which is the energy element.

```
BW[[2]] // MatrixForm
```

This gives the second element the wavefunction in a matrixform.

```
BWProcess[BW]
```

The energy data can be directly called by this command:

```
BWProcess[BW, Output -> "WaveFunction"] // MatrixForm
```

The wavefunction data can be directly displayed through this syntax.

### 3.3 Features

This section takes a deeper look into the features of the BendeWu package. To use the package, it is imperative to know about the feature called “Options”. The outputs of the code can be large, messy and difficult to understand. And that is why the “Option” feature, whose job is to make the output understandable to the users is extremely important to know about and master.

The feature can be used from making the the output truncated to plotting the data in a way to quickly understand the level dependence. It is worth the time and labour to check out the many different options available in both the `BenderWu` function and the `BWProcess` function, and experiment with there results.

#### 3.3.1 Options

The basic syntax of the `BenderWu` function is:

```
BenderWu[V(x), x, (Level Number, (Order), Options]
```

This syntax includes a feature called “Options” which can be used in numerous ways. The options are called with the standard Mathematica syntax:

(Option)->(Option Value)

These options help the user determine how the output is presented. For this they are called “Visualization options”. There are a number of options that can be used to present the output in matrix form or in an array or in a series form.

There are options which can be used to hide the progress monitor which appears when conducting an ongoing calculation. It can be done using the option *Monitor* - > “*False*”. There are options which can be used to output only the energy data or only the wavefunction data.

The options are mentioned in the Table-(3.1).

Options	Results
<i>Monitor</i> - > “ <i>False</i> ”	Turns off progress monitor
<i>OutputStyle</i> - > “ <i>Series</i> ”	To change the output into series
<i>Order</i> - > <i>n</i>	<i>n</i> specifies the order at which to trim the output
<i>Output</i> - > “ <i>Wavefunction</i> ”	to output the wavefunction series
<i>Simplify</i> - > “ <i>True</i> ”	simplifies the analytic expressions at each step
<i>Simplify</i> - > “ <i>False</i> ”	Turning this on may speed up analytic evaluations
<i>Evaluation</i>	Evaluate numerically
<i>WorkingPrecision</i>	Using hardware machine for numerical evaluation
<i>Coupling</i> - > <i>g</i>	A symbol to be used for coupling in output
<i>OutputStyle</i> - > “ <i>Ratio</i> ”	Affects only the “Energy” output.
<i>OutputStyle</i> - > “ <i>RatioPlot</i> ”	Affects only the “Energy” output.

Table 3.1: Visualization options

Some of the options are shared by the functions `BenderWu` and `BWProcess`. These options are presented in Table-(3.2).

<i>Output</i> – > “ <i>Energy</i> ”	output energy
<i>OutputStyle</i> – > “ <i>Array</i> ”	output as array
<i>OutputStyle</i> – > “ <i>Series</i> ”	display the output as a series in the coupling
<i>OutputStyle</i> – > “ <i>Matrix form</i> ”	display output as a matrix
<i>SeriesOutput</i> – > “ <i>Coupling</i> ”	group coupling in wavefunction
<i>SeriesOutput</i> – > “ <i>Argument</i> ”	group powers of argument $x$ in wavefunction

Table 3.2: Options in `BWProcess` function

Most options are shared between the two functions `BWfunction` and `BWProcess` function. If no options are called in the `BenderWu` function, or only evaluation options are called, the default output is in terms of raw data which serves as an input to the `BWProcess` function.

### 3.3.2 Reconstructing level number dependence

Another function of the package `BenderWu` is the `BWLevelPolynomial` function, which allows one to compute the functional form of the energy correction  $\epsilon_{2n}$  on a given level number.

What the function `BWLevelPolynomial` does is, it takes a two-dimensional array, with first level entries of the energy series coefficients  $\epsilon_{2n}$  up to some order  $n_{max}$ , for various level numbers of the potential  $V(x)$ , and returns an array of the polynomials in  $V$  corresponding to each order of  $n = 0, 1, \dots, n_{max}$ .

## 3.4 Utility of the code in various fields

Here is a short summary of all the usages of the code in various fields of physics and also some of the other features of the package that have not been mentioned in this chapter.



1. Quick computation of higher order of perturbation theory.
2. The `BenderWu` package can calculate the first 100 corrections of the perturbation for the potential:

$$\frac{v(gx)}{g^2} = \frac{x^2}{2} + g^2 x^4 \quad (3.10)$$

3. The `BenderWu` function calculates the solution to differential equation:

$$-\frac{1}{2}\Psi''(x) + \frac{1}{g^2}V_0(gx)\Psi(x) + V_2(gx)\Psi(x) = \Psi(x) \quad (3.11)$$

as a perturbation series in the coupling  $g$ .

4. `BenderWu` package can be used to compute energy data and display the wave function of a double well potential which is defined as:

$$V(x) = \frac{x^2(x-1)^2}{2} + v_0 \quad (3.12)$$

5. By implementing the `BenderWu` package we can get the energy data of the supersymmetric double well potential given by:

$$\frac{1}{2}W'(x)^2 + \frac{1}{2}W''(x) \quad (3.13)$$

Which can be given the form:

$$\frac{1}{g^2}V(xg) + V_f(xg) \quad (3.14)$$

6. The `BenderWu` function can handle any potential as long as it has a polynomial power series around  $x = 0$ .

It can be applied on the Jacobi-elliptic potential using the command:

```
BW = BenderWu[JacobiSN[x, m]^2, x, 3, 10, Simplify
-> True];
```

```
BWProcess[BW, Order -> 6]
```

7. The Package can also be used to establish the Sine-Gordon level dependence of perturbation series.

Using the commands:

```
BW3 = Table[BenderWu[Sin[x]^2/2, x, nu, 5, Output
-> "Energy", Monitor -> False], {nu, 0, 7}];
```

```
BW3levels = BWLevelPolynomial[BW3]
```

8. As the potential can be allowed to depend on arbitrary symbolic variables, the study of parametric dependence of perturbation theory can be done.

The `BWDifference` function computes the perturbative expansion of the eigenvalue problem:

$$h(x, p)[\Psi](x) = E[\Psi](x) \quad (3.15)$$

The series expansion of  $x$  and  $E$  can be computed using the command:

```
BW = BWDifference[X + P + 1/X + 1/P, {X, P}, 2, 10];
```

Where,  $h = X + P + 1 = X + 1 = P$ .

9. The higher order perturbative data gained through this code can be used to extract non-perturbative information. This is because of the relation between higher order perturbative data and non-perturbative physics, also known as resurgence.
10. For the reason mentioned in the previous point, it can be used as a teaching tool in the study of resurgence.

## Chapter 4

# Implementation of the code in the derivation of Hawking radiation

Along with all the potentials which have been computed in the previous chapter, we also have implemented it on the potential of the form:

$$2wV = \frac{1}{4} \left[ \ln \left( \frac{w - \frac{r-2M}{r}}{\frac{r-2M}{r}} \right) \right]^2 \quad (4.1)$$

and,

$$V = \frac{1}{8w} \left[ \ln \left( \frac{w - \frac{r-2M}{r}}{\frac{r-2M}{r}} \right) \right]^2 \quad (4.2)$$

Here,  $m$  = mass of black hole, and  $w$  = energy.

Hawking radiation can be thought of as a tunnelling phenomena in Black holes. The black-body radiation is predicted to be released by black hole due to quantum effects near the event horizon. Classically speaking, a particle inside an event horizon cannot escape. But negative energy just beneath the event horizon can escape quantum mechanically and this causes pair production to occur

In the paper written by Wilczek and Parikh, which is named “*Hawking radiation as Tunneling*”, they consider two scenarios of pair creation. First is that the pair production occurs just outside the horizon and the negative

energy particle tunnels in, the positive particle is radiated out. [Figure 4.1]

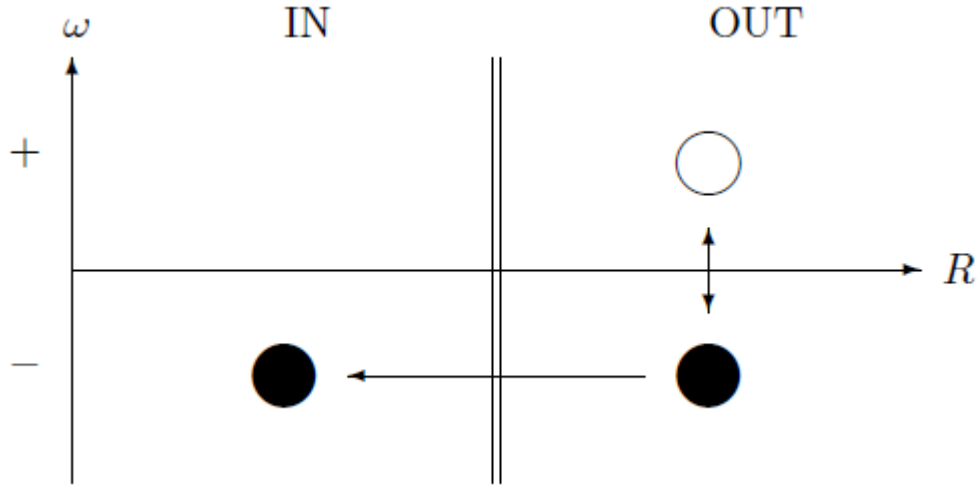


Figure 4.1: Pair creation outside the horizon.

Or, the pair production can occur just inside the horizon with the positive particle tunnelling out. [Figure 4.2] [3] [4]

Wilczek and Parikh show a direct derivation of Hawking radiation as a tunneling phenomena using dynamical geometry and respecting conservation of energy. Tunneling process is treated semi- classically, with the transmission coefficient  $\Gamma$  determined by WKB methods.

The WKB method gives the transmission coefficient or the semi-classical transmission rate:

$$\Gamma = e^{-2ImS} \quad (4.3)$$

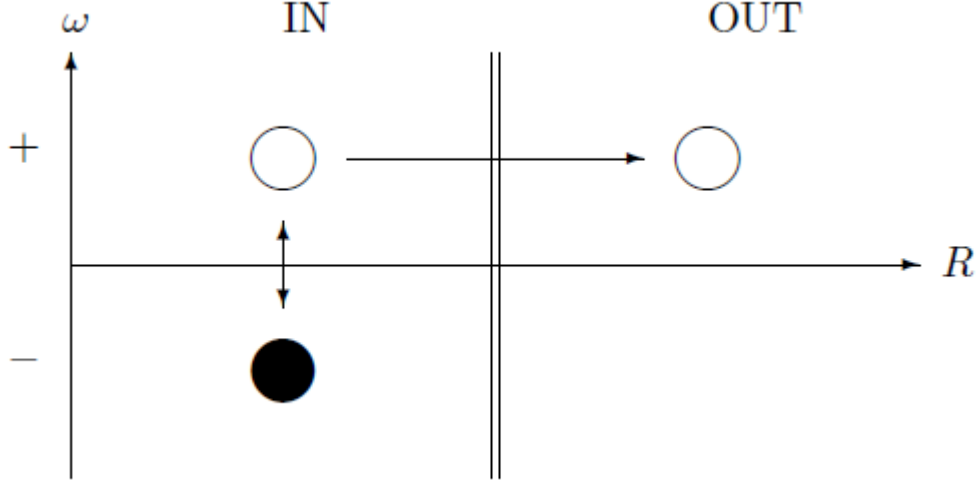


Figure 4.2: Pair production inside the horizon.

Where  $\text{Im } S$  is the imaginary part of the momentum of the outgoing positive particle. This imaginary part is calculated by Wilczek and Parikh. [3]

Wilczek and Parikh calculated  $\text{Im } S$  for a black hole with no charge to be:

$$\text{Im}S = -\text{Im} \left[ \int_0^w \int_{r_{in}}^{r_{out}} \frac{dr}{1 - \frac{\sqrt{2(M-w')}}{r}} \right] \quad (4.4)$$

The interpretation of  $S$  in the WKB formalism is that the transition coefficient  $T$  is:

$$T = e^{i(\text{Re}(S) + i\text{Im}(S))} \quad (4.5)$$

and therefore for metastable decay, the decay rate is:

$$\Gamma = |T|^2 = e^{-2\text{Im}(S)} \quad (4.6)$$

where,

$$\text{Im}S = \int dx \sqrt{2m(V - E)} \quad (4.7)$$

If,  $E = 0$  then,

$$ImS = \sqrt{2m} \int dx \sqrt{V} \quad (4.8)$$

We wish to find the potential  $V$  corresponding to Hawking Radiation. We will then calculate the energy levels for this potential using the Bender-Wu code.

For simplicity, let  $w = m$ . Therefore:

$$\begin{aligned} \sqrt{2w} \int \sqrt{V} dr &= - \int_{r_{in}}^{r_{out}} dr \int_0^w \frac{dw'}{1 - \frac{\sqrt{2(M-w')}}{r}} \\ &= \int_{r_{in}}^{r_{out}} \int_0^w \frac{dw'}{1 - \frac{\sqrt{2(M-w')}}{r}} \end{aligned} \quad (4.9)$$

where,

$$r_{in} = 2M \quad (4.10)$$

$$r_{out} = 2(M - w) \quad (4.11)$$

and we take the limit  $\infty \rightarrow 0$  at the end. This corresponds to a potential barrier of width  $2w$ .

We now approximate the integral is:

$$1 - \sqrt{\frac{2(m-w')}{r}} \approx \frac{1}{4M} (r - 2(M-w')) \quad (4.12)$$

Therefore,

$$ImS = \frac{1}{4M} \int_{r_{out}}^{r_{in}} dr \int_0^w \frac{dw'}{r - (M - w')} \quad (4.13)$$

Now,

$$\begin{aligned}
\int_0^w \frac{dw'}{r - 2(M - w')} &= \int_0^w \frac{dw'}{2w' - 2M + r} \\
&= \frac{1}{2} \int_0^w \frac{dw'}{w' + \frac{r-2M}{2}} \\
&= \frac{1}{2} \ln \left( w' + \frac{r-2M}{2} \right) \Big|_0^w \\
&= \frac{1}{2} \ln \left( \frac{w + \frac{r-2M}{2}}{\frac{r-2M}{2}} \right)
\end{aligned}$$

Therefore,

$$\sqrt{2w} \int \sqrt{V} dr = \frac{1}{2} \int dr \ln \left( \frac{w + \frac{r-2M}{2}}{\frac{r-2M}{2}} \right) \quad (4.14)$$

The potential is therefore:

$$2wV = \frac{1}{4} \left[ \ln \left( \frac{w - \frac{r-2M}{r}}{\frac{r-2M}{r}} \right) \right]^2 \quad (4.15)$$

$$V = \frac{1}{8w} \left[ \ln \left( \frac{w - \frac{r-2M}{r}}{\frac{r-2M}{r}} \right) \right]^2 \quad (4.16)$$

Now, we use the Bender-Wu code to find the energy eigenvalues. We will replace  $w$  with  $x$  in the code.

To execute the code on the potential in the Equation-4.16, to find the energy eigenvalues at the energy level = 2 and up to the first order, we first define the potential to Mathematica using:

$$V[x] := (1/4) (\text{Log}[\frac{(x - ((r - 2 m)/r))}{((r - 2 m)/r)}])^2$$

Then, to calculate the potential, we use the command:

$$\text{BW} = \text{BenderWu}[V[x], x, 2, 1];$$





So, the energy eigenvalue:

$$\epsilon = \frac{5}{2} \sqrt{V'''[0]} + \dots$$

And, to execute the code on the potential in equation-4.17, first we define the potential in Mathematica:

$$V[x] = (1/8 x) \{ \text{Log}[(x - ((r - 2 m)/r))/((r - 2 m)/r)] \}^2$$

Then, to calculate the energy data at the third energy level and up to the fourth order, we use the command:

`BW = BenderWu[V[x], x, 3, 4, Output -> "Energy"];`

Which returns the data:

$$\left\{ \frac{7}{2} \sqrt{V''[0]}, -\frac{7V^{(3)}[0]^2}{36V''[0]^2} - \frac{5}{2} \left( -2 \left( \frac{7V^{(3)}[0]^2}{12V''[0]^2} - \frac{V^{(4)}[0]}{16V''[0]} \right) + \frac{21}{4} \left( \frac{V^{(3)}[0]^2}{9V''[0]^2} - 2 \left( -\frac{7V^{(3)}[0]^2}{72V''[0]^2} + \frac{V^{(4)}[0]}{24V''[0]} \right) \right) \right), \frac{V^{(3)}[0]}{36V''[0]} - \frac{5}{2} \frac{V^{(4)}[0]}{V''[0]}, \frac{1}{V''[0]^{3/2}} \left( \frac{V^{(3)}[0]}{36V''[0]} - \frac{5}{2} \left( \frac{1}{2} \left( \frac{V^{(3)}[0]}{36V''[0]} \left( \frac{28V^{(3)}[0]}{3V''[0]} - 6 \right) - \frac{5}{2} \left( \frac{1}{2} \left( -2 \left( \dots \right) + \dots \right) \left( -\frac{7}{36} \dots^2 - \frac{5}{2} \left( -2 \left( \dots \right) + \frac{21}{4} \dots \right) \right) - \dots \right) \right) \right) \right\}$$

Here, many of the values are omitted. If the values are too large to fit in the screen, the software keeps it omitted. It can be displayed fully if it is

instructed to show more of the result.

The energy eigenvalue as series:

$$\epsilon = \frac{7}{2}\sqrt{V''[0]} - \frac{7V^5[0]^2}{36V''[0]^2} - \dots$$

The interpretation of these eigenvalues is left for future work.

# Chapter 5

## Non-Perturbative physics, Resurgence

In Quantum physics there are few problems which are exactly solvable. For this reason approximation methods are a big part of application of theories and so are the problems whose exact solutions are available. These exact solutions start as a starting point for approximation methods.

The Perturbation theory is one such approximation method which is concerned with finding the changes in the discrete energy levels and eigenfunctions of a system when a small disturbance is applied. The solution is based upon the exact solution of the systems, when there is no disturbance in the system.

The perturbation of Hamiltonian for example is of this form:

$$H = H_0 + \lambda H' \tag{5.1}$$

Where  $H_0$  is unperturbed Hamiltonian,  $H'$  is perturbed Hamiltonian, and  $\lambda$  is small parameter. [10]

Perturbation theory has been hugely useful in theoretical problems. However, it does have its limitations. For example perturbative solutions can only be for systems with weak coupling. Systems with strongly interacting

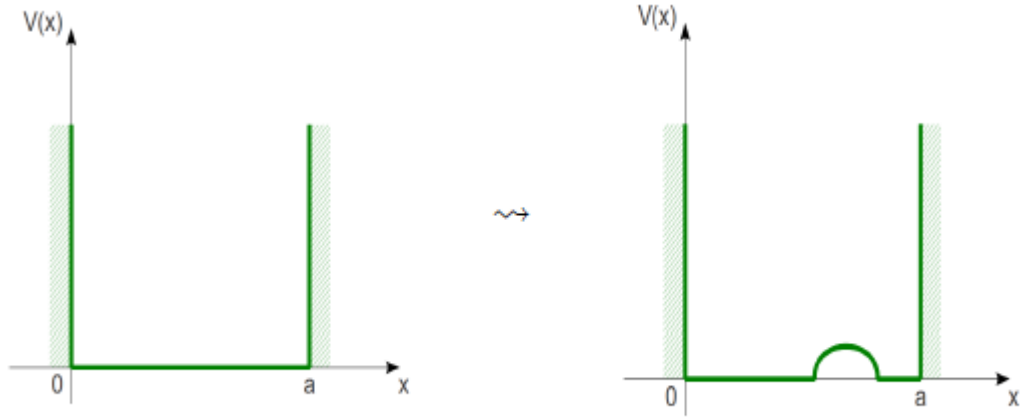


Figure 5.1: An unperturbed potential well, and a slightly perturbed potential well (right).

particles do not have useful perturbative solutions. And these systems are in plenty in physics. For these cases non-perturbative solutions are appropriate. Non-perturbative solutions offer more accurate description to these systems along with offering new insights that perturbation theory cannot offer.

A function or a problem that cannot be accurately described by perturbation theory is called non-perturbative. Non-perturbative solutions can offer insights that perturbative solutions cannot. Some examples of non-perturbative approximation methods are: Lattice QCD, Anti-de Sitter/QCD. Solitons and Instantons are non trivial solutions to Quantum field theory which are perturbative in nature.

The behavior of higher order perturbation theory has been a topic of research due to its interesting characteristics. It was Dyson who first suggested that perturbation expansion in QED should be divergent. Later with works from C. A. Hurst and W. Thirring , and A. Petermann through computation, showed that perturbation expansion in higher order is divergent. Later in Arkady's work, he gave quantitative statement of the relation between this large order divergence of perturbative coefficients and non perturbative physics.

In terms of non-perturbative physics, instantons are a critical concept. Instantons are classical solutions to the Wick rotated equations of motion which have non-trivial topology. They are useful in both Quantum mechanics and Quantum Field Theory. While in Quantum Mechanics, they are used to describe tunneling/decay phenomena by using a semi-classical approximation to equations of motion with imaginary time, in Quantum Field Theory, instantons are described by gauge fields with non-trivial winding at infinity. There also they lead to a description of tunneling and decay. [6]

## 5.1 Relation between perturbative and non-perturbative physics

There are interesting relations between perturbative and non-perturbative physics, and this interconnections have been the focus of research for many papers. In this section some of the aspects of these works are summarized.

For quantum potentials, the perturbative data of their fluctuations, lead to non-perturbative data in higher non-perturbative sectors. These quantum potentials include instanton examples of periodic cosine and symmetric double well potentials.

One of the characteristics of resurgent behaviour is that fluctuations about all non-perturbative sectors are encoded in the perturbative expansion about the vacuum sector. This is considered a constructive form of resurgence and is observed in formulas for the ionization rate of Hydrogen atoms. They are also observed in periodic cosine Mathieu potentials and supersymmetric Mathieu potentials.

This constructive resurgence has the form:

$$-\frac{\hbar^2}{2} \frac{d^2}{dx^2} \psi + V(x)\psi = u\psi \quad (5.2)$$

Which is the Schrodinger equation with the energy  $u$ . We can consider the energy perturbative series  $u_{pert}(\hbar, N)$ , where,  $\hbar$  is the coupling and  $N$  is the unperturbed harmonic energy level. The perturbative data  $u_{pert}(\hbar, N)$

can be used to write an constructive expression for the fluctuation about any higher order non-perturbative sector.

To demonstrate this, the Mathieu cosine potential,  $V(x) = \cos^2 x$ , the edges of the  $N$ th band are given by the trans-series expression:

$$u(\hbar, N) = u_{pert}(\hbar, N) + \sqrt{\frac{2}{\pi}} \frac{1}{N!} \left(\frac{2^{7/2}}{\hbar}\right)^{N+1/2} \exp\left[-\frac{2\sqrt{2}}{\hbar}\right] P_{inst}(\hbar, N) \quad (5.3)$$

Both the perturbative series  $u_{pert}(\hbar, N)$  and the one-instanton sector  $P_{inst}(\hbar, N)$  are divergent series.

In the Mathieu system perturbative/non-perturbative relation results in the suppression of the one-instanton term in the trans-series. The non-perturbative one-instanton term in trans-series including all orders fluctuation factor  $P_{inst}(\hbar, N)$  is expressed through perturbative data:

$$P_{inst}(\hbar, N) = \frac{\partial u_{pert}(\hbar, N)}{\partial N} \exp\left[\frac{S_I}{w_c} \int \frac{d\hbar}{\hbar^3} \left(\frac{\partial u_{pert}(\hbar, N)}{\partial N} - \hbar w_c + \frac{\hbar^2 w_c (N + 1/2)}{S_I}\right)\right] \quad (5.4)$$

Where,  $u_{pert}$  is the perturbative expansion term. In terms of genus-1 systems as well, non-perturbative information is coded in perturbative expansion. Here,  $S_I = 2\sqrt{2}$  in the one-instanton action and  $w_c = \sqrt{2}$  is the classical frequency for the harmonic motion which is at the bottom of the potential well for the Mathieu potential,  $V(x) = \cos^2 x$ .

The equation-5.2 shows that, all  $\hbar$  dependent factors in equation-5.3 are encoded in  $u_{pert}(\hbar, N)$ , which is a perturbative series. Thus, giving the example of a constructive resurgence. [5]

The decoding of these non-perturbative information from perturbative expansion can be done by perturbation theory being combined with a global boundary condition that specifies how one degenerate vacuum connects to another. This technique works for a wide variety of degenerate vacua potentials, such as double well potential and the periodic Sine-Gordon potential. The

entire trans-series, to all nonperturbative orders, can be encoded in terms of just the perturbative saddle point, because the fluctuations about different saddle points are tightly related.

Studying the behavior of perturbation theory in higher order also reflects on this relation. The field theory perturbation series in the renormalised coupling is divergent, and the reason for this is instantons. The IR ambiguities in perturbative QCD are associated with non-logarithmic UV divergences in the non-perturbative Operator Product Expansion (OPE), and can cancel between the perturbative and non-perturbative sectors. There is also a connection between the large-order behavior of quantum mechanical perturbation theory and WKB methods which was developed by Bender and Wu.

In fact there are many examples in physics where divergence in perturbation theory can be associated with potential instability and thus provide link between perturbative and non-perturbative physics. There is a precise quantitative relation between the large-order divergence of the perturbative coefficients and non-perturbative physics.

This instability and its relation to perturbation was described by Arkady in his paper “*Decaying systems and divergence of perturbation theory*”. He considers the  $\phi\lambda^3$  theory in quantum mechanics and consider it for the Hamiltonian:

$$H = \frac{1}{2}\phi'^2 + \frac{1}{2}m^2\phi^2 - \lambda\phi^3 \tag{5.5}$$

He also takes the unstable ground state  $|\psi\rangle$ . One of the main outcomes from his paper was that divergence of perturbation theory is related to instability in the theory. And divergence of perturbative coefficients is related to non-perturbative physics. [7]

## 5.2 Resurgence

Resurgence theory is a formalism that unifies perturbative and nonperturbative physics. It has application in QM, QFT and String theory.

The concept of Resurgence was mostly worked on during the 1980s by the mathematician Jean Ecalle. Then its usage spread to theoretical physics as well. Also, contribution in this notion has been made by J. Zinn-Justin, M. Berry, U. Jentschura, G. Dunne, M. Beneke.

One other notion related to resurgence is trans-series. Trans-series can roughly be called an expansion for real valued functions. It has become important in asymptotic analysis, model theory, computer algebra.

In terms of quantum spectral problems, two distinct type of resurgent behavior has been identified. One is the “Large order/ low order” behavior where large order of expansion of perturbative coefficient about non-perturbative sector is related to low order of perturbative coefficients of fluctuations about other non-perturbative sectors. Another is the “low order/low order” behavior where fluctuations about non-perturbative sectors are encoded in perturbative expansion around vacuum sector.

Resurgence faces conceptual difficulties in strongly coupled Yang-mills theories, if it is carried out in the same way as in quantum mechanics. A way to get around it may be to use Wilson’s operator product expansion (OPE) adapted to QCD, which has conceptual similarities with the resurgence program.



# Chapter 6

## Conclusion

The significance of the BenderWu Mathematica package in the world of computation and physics, is in its accessibility and ease of use. Anyone can use it from the comfort of their home. In the present state of physics it is imperative to incorporate computational methods in all its branches. That is why this field needs a significant number of researchers skilled in these techniques. The resources in universities might not be enough to meet this increasing demand. That is why it is important to develop codes that can be implemented using Wolfram Mathematica, Python and other resources that can be accessed through home computer.

The code is also important because it can be used in a variety of different potentials. In this thesis we have applied it to potentials of polynomial form, trigonometric form, and potential related to tunneling. The generality of the code that can be translated to use in a variety of different potentials, makes it extremely useful.

The contribution of this code to the field of resurgence is of immense value as well. The field of resurgence is rapidly growing and to understand the relation between higher order perturbative data and non-perturbative theory this code can be very useful. It can be used in decoding non-perturbative data from perturbative expansion, as well as contribute to the understanding of the behaviour of higher order perturbation series, and its connection to tunneling.

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