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Usual and Unusual Perturbative Expansion Parameters in Quantum Mechanics

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Abstract

This report briefly introduces perturbation theory and discusses the divergence of perturbation series and how to deal with it using Padé Summation. Then it explores the $\frac{1}{N}$ expansion method in Quantum mechanics. In particular, two different methods to obtain the coefficients of this expansion are explained using the Hydrogen atom as an example. This method is then validated by looking at the results that it provides for different physical systems and comparing them with literature values. Finally, the $\frac{1}{N}$ expansion is used to analyse the energy levels of the Yukawa potential in great detail.

Declaration

I declare that this project and report is my own work.

Signature: Date: 31/03/2023

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1 Introduction

The need for approximations is at the very core of Physics and is particularly important in Quantum Mechanics. Unfortunately, exactly solvable problems are rare in the context of Quantum mechanics and the Schrodinger Equation. Even for simple-looking systems such as the anharmonic oscillator $V(x) = \frac{1}{4}x^2 + \frac{1}{4}\lambda x^4$ the Schrodinger Equation cannot be solved exactly.

Therefore, several techniques have been developed to obtain approximate solutions for the SE over the years. Perturbation Theory is a particularly successful strategy in this context, which allows us to decompose a seemingly difficult problem into an infinite set of recursively easy ones [1].

1.1 Perturbation Theory

1.1.1 Mathematical Formalism

Perturbation theory in mathematics is a collection of techniques that allows us to get approximate solutions to hard problems that are difficult (or impossible) to solve exactly [1]. In general, all perturbation problems can be summarized in three steps:

1. Introduce a parameter λ
2. Assume that the solution to the problem takes the form of $\sum_{n=0}^{\infty} a_n \lambda^n$ and get the coefficients
3. Sum the series to get the result

In particular, in the context of quantum mechanics, perturbation theory is used to solve the eigenvalue problem of the form:

$$\left(-\frac{d^2}{dx^2} + V(x) + \lambda W(x)\right)\psi(x) = E\psi(x) \tag{1}$$

With the additional boundary condition of $\psi(x) \to 0$ as $|x| \to \infty$, we assume that we can solve the problem $\left(\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\psi(x)$ subject to the same boundary conditions [1].

Therefore, we seek solutions to both the eigenfunctions and the eigenvalues as power series in λ. That is, we need to find the coefficients of:

$$E_n = \sum_{n=0}^{\infty} E_n \lambda^n \tag{2}$$

$$\psi(x) = \sum_{n=0}^{\infty} \psi_n(x) \lambda^n \tag{3}$$

Therefore, we just have to find all the coefficients and then sum the series to obtain an answer to the problem. While the problem of getting the coefficients might seem more difficult at first sight, there are standard techniques to obtain them [1], and the real problem usually comes in summing the series.

1.1.2 Divergence of Perturbation Theory

While Perturbation theory in Quantum Mechanics is taught ubiquitously at an undergraduate level, it is usually not explained that perturbation series usually have a zero radius of convergence, meaning that they diverge for all values of λ. Formally that means that the sequence of partial sums

$$E(\lambda, N) = \sum_{n=0}^{N} a_n \lambda^n \tag{4}$$

does not have a limit (S) for any value of λ.

The fact that the perturbation series diverges is closely related to the underlying analytic structure of the function $E(\lambda)$ in the complex λ plane [1]. In particular, if $E(\lambda)$ has a sequence (infinite) of branch points with a limit point in the origin, the perturbation series will have a zero radius of convergence [1]. This is precisely what happens in the case of the Anharmonic Oscillator [2]. A more detailed explanation of the divergence of perturbation theory and how to analyse the analytic structure of $E(\lambda)$ in the complex plane can be found in Reference [1].

1.2 Dealing with the Devil

In 1828 Abel said, "Divergent series are the invention of the devil, and it is shameful to base them on any demonstration whatsoever". If, as explained in the previous section, perturbation series in Quantum mechanics usually have a zero radius of convergence, then the natural question is: Why are we using them?

Once we know that the perturbation series $\sum_{n=0}^{\infty} a_n \lambda^n$ diverges, we can no longer say that this series is equal to the Energy eigenvalue. Still, it is true that the Energy eigenvalue is asymptotic to the perturbation expansion [1]:

$$E(\lambda) \sim \sum_{n=0}^{\infty} a_n \lambda^n \tag{5}$$

Therefore, when we find a divergent series using perturbation theory, we really find an asymptotic representation of the function $E(\lambda)$. Many powerful methods have been developed to extract the correct answer ($E(\lambda)$) with arbitrary precision from its asymptotic representation when given by a divergent series [3]. We will now introduce one of these methods, the Padé Approximant, as it will be relevant to the project.

1.2.1 Padé Summation

Let us assume that we have a function $f(z)$ represented by the power series $\sum_{n=0}^{\infty} a_n z^n$, which might be divergent. We construct the Padé approximants ($P_M^N(z)$) as the ratio of two polynomials.

$$P_M^N(z) = \frac{\sum_{n=0}^{N} A_n z^n}{\sum_{n=0}^{M} B_n z^n} \tag{6}$$

Additionally, It is possible to choose $B_0 = 1$ without loss of generality. Then, the remaining coefficients (there are $M + N + 1$ of them left to determine) are chosen such that the first $M + N + 1$ coefficients of the Taylor expansion of the resulting Padé Approximant match the first $M + N + 1$ coefficients of the sum $\sum_{n=0}^{\infty} a_n z^n$.

In many cases, it is found that $P_M^N(z) \to f(z)$ in the limit $M, N \to \infty$ even if the original power series that represents $f(z)$ is divergent [3]. Therefore, we can try to use the Padé Approximants to approximate the function represented by the initial power series. There are stills many unknowns in the general convergence properties of the Padé Approximants [3]. However, this method has been successfully applied in Quantum mechanics. For instance, it has been applied to the perturbation series of the Yukawa potential [4]. This section is just meant to briefly introduce the method of Padé Summation, a more in-depth study of the method can be found in Reference [3].

2 The $\frac{1}{N}$ Expansion in Quantum Mechanics

We will now introduce The $\frac{1}{N}$ expansion, an alternative analytic method to traditional perturbation theory that can be used to obtain approximate solutions to the Schrodinger Equation. Instead of using the coupling constants of the potentials as expansion parameters, we will use the number of dimensions as the expansion parameter. It has the advantage of not requiring the Hamiltonian to be given as a sum of a solvable part and a perturbation. However, before examining how such expansion can be generated, we must analyse how the Schrodinger Equation is formulated in N dimensions.

2.1 Schrodinger Equation in N Dimensions

The Time independent Schrodinger Equation can be expressed as

$$\hat{H}\Psi(\underline{r}) = E\Psi(\underline{r}) \tag{7}$$

Where $\hat{H}$ is the Hamiltonian of the system and $\Psi(\underline{r})$ is an eigenfunction of this operator with eigenvalue E. Assuming atomic units ($\hbar = m = 1$), it is possible to express the Hamiltonian in N dimensions as:

$$\hat{H}_N = -\frac{\nabla_N^2}{2} + \hat{V}_N \tag{8}$$

N denotes the number of dimensions, $\hat{V}_N(\underline{r})$, is the potential in N dimensions and ∇_N^2 is the N-dimensional Laplacian operator. In Cartesian coordinates, the N-dimensional Laplacian and the position vector are defined in the usual manner:

$$\nabla_N^2 = \sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} \qquad\qquad \underline{r} = \sum_{i=1}^{N} x_i \underline{e}_i \tag{9}$$

While Cartesian coordinates might appear more attractive, (hyper)spherical coordinates turn out to be more useful if the potential is (hyper)spherically symmetric[1]. Therefore we

[1]Meaning that the potential only depends on the modulus of the position vector

move from the usual Cartesian coordinates $\{x_i, i = 1, ..., N\}$ to hyperspherical coordinates $\{\theta_i, i = 0, ...N-1\}$ in which we identify $\theta_0 = r$. It is possible to express the N-dimensional Laplacian operator in terms of this new set of coordinates [5]

$$\nabla_N^2 = \frac{1}{h}\sum_{i=0}^{N-1}\frac{\partial}{\partial\theta_i}\frac{h}{h_i^2}\frac{\partial}{\partial\theta_i} \ , \ h_i^2 = \sum_{j=1}^{N}\left(\frac{\partial x_j}{\partial\theta_i}\right)^2 \ , \ h = \Pi_{i=0}^{N-1}h_i \tag{10}$$

The Angular momentum components L_{ij} are defined as:

$$L_{ij} = -L_{ji} = x_i p_j - x_j p_i, i = 1, 2, ..., j-1, j = 2, 3..., N \tag{11}$$

In Equation 11, p_i is the momentum operator canonically conjugate to x_i and it is defined as $p_i = -i\frac{\partial}{\partial x_i} =$ [5]. Expressing the momentum operators in terms of the hyperspherical coordinates is also possible $p_k = -i\sum_{j=0}^{N-1}\frac{1}{h_j^2}\frac{\partial x_k}{\partial\theta_j}\frac{\partial}{\partial\theta_k}$ [5]. There are a total of $\frac{N(N-1)}{2}$ components of the angular momentum tensor, and these are the generators of rotations in N dimensions, and they form the basis of the Lie Algebra of the O(N) group [5]. For example, in 3 dimensions, there are three components of the angular momentum L_{12}, L_{13} and L_{23}, which correspond to the usual L_z, L_y and L_x respectively.

At this stage, it is useful to introduce the Casimir invariants, which are defined as follows:

$$L_k^2 = \sum_{j=2}^{k+1}\sum_{i=1}^{j} L_{ij}L_{ij}, k = 1, ..., N-1 \tag{12}$$

In the case $N = 3$ there are only two of these operators, L_1^2 and L_2^2, which correspond to the usual L_z^2 and $L^2 = L_x^2 + L_y^2 + L_z^2$ respectively [6]. It can be shown (see Ref [5] for a complete explanation) that the Laplacian operator in N dimensions can be expressed in terms of the radial component and L_{N-1}^2 in the following way:

$$\nabla_N^2 = \frac{\partial^2}{\partial r^2} + \frac{N-1}{r}\frac{\partial}{\partial r} - \frac{L_{N-1}^2}{r^2} \tag{13}$$

Given that the Casimir Invariants commute with each other it is possible to find a common set of eigenfunctions that we denote as $Y_{\lambda_{N-1},\lambda_{N-2},...,\lambda_1}(\theta_1, \theta_2, ..., \theta_{N-1})$ such that $L_k^2 Y_{\lambda_{N-1},\lambda_{N-2},...,\lambda_1}(\theta_1, \theta_2, ..., \theta_{N-1}) = \lambda_k Y_{\lambda_{N-1},\lambda_{N-2},...,\lambda_1}(\theta_1, \theta_2, ..., \theta_{N-1})$. Furthermore, it is possible to show (see Ref [5] for more details) that $\lambda_k = l_k(l_k + k - 1)$ where l_k is an integer and that once l_k has been chosen l_{k-1} can only take values from 0 to l_k. Therefore, it is possible to label the eigenfunctions using the set of integers l_k [5].

$$Y_{\lambda_{N-1},\lambda_{N-2},...,\lambda_1}(\theta_1, \theta_2, ..., \theta_{N-1}) \rightarrow Y_{l_{N-1},l_{N-2},...,l_1}(\theta_1, \theta_2, ..., \theta_{N-1}) \tag{14}$$

$$L_k^2 Y_{l_{N-1},l_{N-2},...,l_1}(\theta_1, \theta_2, ..., \theta_{N-1}) = l_k(l_k + k - 1)Y_{l_{N-1},l_{N-2},...,l_1}(\theta_1, \theta_2, ..., \theta_{N-1}) \tag{15}$$

The set of functions $Y_{l_{N-1},l_{N-2},...,l_1}(\theta_{N-1}, \theta_{N-2}, ..., \theta_1)$ are known as generalized spherical harmonics [5]. In our particular case in which k goes up to $N-1$, l_{N-1} can go from 0 to ∞ and l_{N-2} from 0 to l_{N-1} and so on. It is useful to denote l_{N-1} simply as l and L_{N-1}^2 as L^2.

In the case of a spherically symmetric potential, the Hamiltonian of the system commutes with L^2, which means that it is possible to find a complete set of eigenfunctions that are simultaneously eigenfunctions of $\hat{H}_N$ and L^2. Therefore it is sensible to express $\Psi(\underline{r})$ as:

$$\Psi(\underline{r}) = R(r)Y_{l,l_{N-2},...,l_1}(\theta_1, \theta_2, ..., \theta_{N-1}) \tag{16}$$

Where $R(r)$ is the radial part of the wavefunction and is still to be determined. If now we substitute Equation 16 into the Schrödingers Equation, it is easy to obtain an equation for $R(r)$:

$$\left[-\frac{1}{2}\left(\frac{d^2}{dr^2} + \frac{N-1}{r}\frac{d}{dr}\right) + \frac{l(l+N-2)}{2r^2} + V_N(r)\right] R(r) = ER(r) \tag{17}$$

Which is the Radial Schrodinger Equation (RSE). In this case, l is used to identify the angular momentum quantum number. It is useful to introduce the function $u(r) = r^{\frac{N-1}{2}}R(r)$ as substituting it into Equation 17 leads to further simplification:

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{(k-1)(k-3)}{8r^2} + V_N(r)\right] u(r) = Eu(r) \tag{18}$$

In which $k = N + 2l$. Equation 18 is the key equation on which the following sections will be based.

2.2 Lowest Order Approximation or the Large N Limit

At this stage, we have expressed the N-dimensional Schrodinger's Equation in simple terms but have yet to make any approximation. Therefore, it is time to start extracting useful information from the equations presented in the section above.

Firstly, it is necessary to carefully set up the problem we are trying to solve. We are interested in solving the Schrodinger Equation for a D (usually D=3) dimensional potential[2], which can be written as $V(r)$. However, instead of directly solving this problem, let us solve a seemingly more complicated and general problem. Let us solve the Schrödinger Equation in N dimensions for a potential V_N that can be written as[3]:

$$V_N(r) = \frac{k^2}{(D+2l)^2}V(r) \tag{19}$$

This problem reduces to the initial problem when $N = D$ (as $k = N + 2l$ as before) and when $N \neq D$, the potential preserves the essence of $V(r)$ (it is $V(r)$ multiplied by some value). The important point is that if we can write a solution for this problem (or an approximate solution), we just have to let $N = D$ at the end of the calculation to get the solution of our original system. The factor of $\frac{1}{(D+2l)^2}$ is usually absorbed by defining: $\bar{V}(r) = \frac{V}{(D+2l)^2}$ [7].

If we want to be completely general with the number of dimensions, we can just $(D+2l) \rightarrow k$ at the end of our calculation. This will produce a result that works for all dimensions simultaneously, but we are usually just interested in the case $D = 3$.

[2]Here, D is just a value, not a parameter

[3]Where N is a parameter, meaning that we have to solve the problem for all N

Note that this choice of N-dimensional problem that we want to solve (mainly how we define $V_N(r)$) is not unique, but we need the problem to reduce to the initial D-dimensional problem when $N = D$; in some instances, other choices might be beneficial [5; 8]. However, using this choice of $V_N(r)$ allows to rewrite Equation 18 as follows:

$$\left[-\frac{1}{2k^2}\frac{d^2}{dr^2} + \frac{(1-\frac{1}{k})(1-\frac{3}{k})}{8r^2} + \bar{V}(r)\right] u(r) = \frac{E}{k^2}u(r) \tag{20}$$

In the large k limit, the eigenfunctions of the system will become peaked towards the value r_0, which is the value that minimizes the leading contribution of the potential $V_{eff}(r) = \frac{1}{8r^2} + \bar{V}(r)$[7], and the energy eigenvalues will tend towards the value [7; 5]

$$E_\infty = k^2 V_{eff}(r_0) \tag{21}$$

r_0 is defined from the condition $\left[\frac{dV_eff}{dr}\right]_{r=r_0} = 0$. For finite N, the value given by E_∞ is only an approximation of the real energy eigenvalue. Given that we are usually interested in three-dimensional cases, the approximation of the Energy by E_∞ does not provide an excellent answer.

At this stage, it is helpful to verify how effective the E_∞ approximation is for the ground state energy of a 3D potential. The Hydrogen atom offers an excellent example as it can be solved exactly. Therefore, the E_∞ approximation can be compared with the exact value of the ground state energy.

Hydrogen Atom
The application of this method to the Hydrogen atom ($V(r) = \frac{-e^2}{r}, D = 3$) results in $E_\infty = \frac{-2e^4k^2}{(D+2l)^4}$ if we want to be completely general with the number of dimensions we can let $D \to N$ giving $E_\infty = \frac{-2e^4}{k^2}$. The Hydrogen Atom can be solved exactly in any number of dimensions, and the exact answer of the Ground State energy in N dimensions is: $E_{\text{Exact}} = \frac{-2e^4}{(N-1)^2}$ [7; 9]. In the 3-dimensional case, our approximation of the ground state (l=0) becomes $E_\infty = \frac{-2e^4}{9}$ [10]. The relative error of this first approximation is 55.5% in the 3-dimensional case. In larger dimensions, the error on the first-order approximation is attenuated.

It is clear that we need to develop a technique to add corrections to E_∞ such that it provides a satisfactory answer for finite N. These techniques will be explained in the following sections.

2.3 Finite N corrections

The discussion above offers the leading term of the $\frac{1}{N}$ expansion. However, this term is often a poor estimate of the real value of the Energy eigenvalues of the system when we set $N = D = 3$. Therefore, this section will delve into how the actual expansion in terms of powers of $\frac{1}{N}$ can be constructed to provide corrections for finite N (usually $N = 3$) and how to do so for both the ground state and excited states.

2.3.1 Riccati Equation

This method can be used to obtain corrections for the ground state energy. At this stage, it is useful to introduce the new coordinate $x = r - r_0$, which leads to the function $g(x) = u(x + r_0)$. Furthermore, it is possible to make the following Ansazt of $g(x)$ [5; 7]:

$$g(x) = e^{\phi_0(x)} \tag{22}$$

This Ansatz gives a nodeless wavefunction (as expected for the ground state)[5]. This Ansatz can now be inserted into Equation 18, and as the first term of the Energy series is already known, it can be subtracted from the expression. After some simplification, the resulting expression is:

$$-\frac{1}{2}\left[\phi_0'(x)^2 + \phi_0''(x)\right] + k^2\bar{V}_{eff} + \frac{3}{8r^2(x)} - \frac{k}{2r^2(x)} = \xi_0 \tag{23}$$

With $\bar{V}_{eff} = V_{eff} - V_{eff}(r_0)$ and $\xi_0 = E - k^2 V_{eff}(r_0)$
This is a Riccati Equation in terms of $\phi_0'(x)$ [5], which gives the name to the method. At this point, it is time to express both $\phi_0'(x)$ and ξ_0 as power series of k.

$$\xi_0 = \sum_{n=-1}^{\infty} E_0^{(n)} k^{-n} \qquad\qquad \phi_0'(x) = \sum_{n=-1}^{\infty} \phi_0^{(n)}(x) k^{-n} \tag{24}$$

These relations can be inserted in Equation 23, and the coefficients of the same power of k can be matched to obtain expressions for all the coefficients. The obtained relations are shown below:

$$\phi_0^{(-1)}(x) = -\sqrt{2\bar{V}_{eff}(x)} \tag{25}$$

$$\sqrt{2\bar{V}_{eff}}\phi_0^{(0)}(x) = E_0^{(-1)} + \frac{1}{2}r^{-2}(x) + \frac{1}{2}\phi_0^{(-1)'}(x) \tag{26}$$

$$\sqrt{2\bar{V}_{eff}}\phi_0^{(1)}(x) = E_0^{(0)} - \frac{3}{8}r^{-2}(x) + \frac{1}{2}\left[\phi_0^{(0)'}(x) + \phi_0^{(0)2}(x)\right] \tag{27}$$

$$\sqrt{2\bar{V}_{eff}}\phi_0^{(n+1)}(x) = E_0^{(n)} + \frac{1}{2}\left[\phi_0^{(n)'}(x) + \sum_{m=0}^{n}\phi_0^{(m)}(x)\phi_0^{(n-m)(x)}\right], \qquad n > 0 \tag{28}$$

The procedure to extract the coefficients from these relations is the following, first $\phi_0^{-1}(x)$ is determined from the expression of the effective potential. Then the next equation is evaluated at $x = 0$ (value for which the effective potential $\bar{V}_{eff}$ vanishes) to obtain $E_0^{(-1)}$. Having an expression for the first coefficient of the Energy is now possible to get $\phi_0^{(1)}(x)$ from the same equation [7; 5]. The process is repeated for each relation until we reach the desired number of coefficients.

Coulomb Potential Example
At this stage, testing the method with the simple case of the Hydrogen Atom is helpful. Figure 1 shows the partial sums $E_0(n) = \sum_{j=-2}^{n} E_0^{(j)} k^{-j}$ as a function of n (the upper limit of the sum). The coefficients of the sum were calculated by implementing the relations in equations [21-24] in Mathematica and using recursion to get the coefficients. Memoization was used to help speed up the calculations of the recursive algorithm.

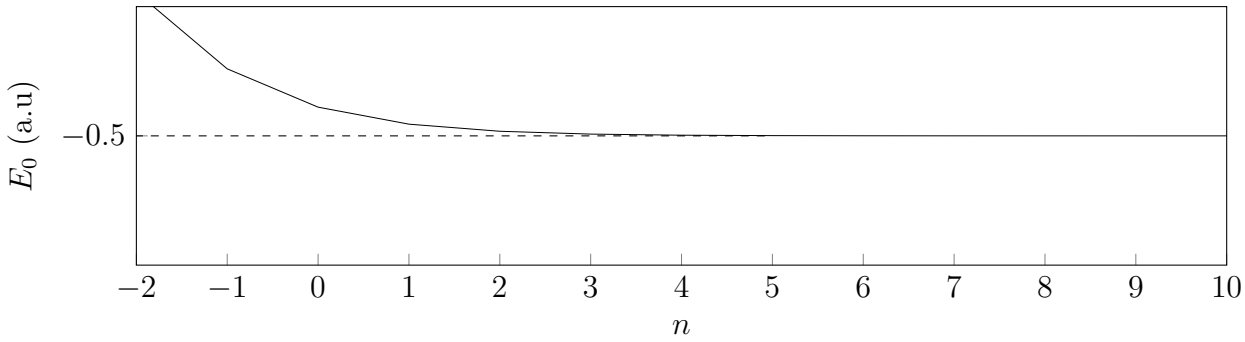

Fig. 1: Partial sums of the $\frac{1}{N}$ Expansion of the Ground State Energy of a particle in a Coulomb Potential, the series converges to -0.5 (in atomic units), which is the exact result of this problem and that value is represented as a dashed line in the plot.

It can be seen from the figure that in the case of 3 Dimensions, the Energy series seems to converge to the correct result (-0.5 in atomic units). The convergence rate is also satisfactory as only a few terms are required to get reasonably close to the correct result (with only six terms, the accuracy of the expansion is 99.3%).

The functions $\phi_0^n(x)$ calculated when getting the Energy coefficients can be used to reconstruct the radial wavefunction [7].

$$\phi'(x) = \sum_{n=-1}^{\infty} \phi_0^n(x) k^{(-n)} \tag{29}$$

$$g(x) = \exp\left\{ \int^x \sum_{n=-1}^{\infty} \phi_0^n(x) k^{-n} \right\} \tag{30}$$

$$R(r) = Cr^{\frac{-(N-1)}{2}} g(x(r)) \tag{31}$$

C is a constant that can be determined by imposing the normalization condition on $R(r)$. The plot in Figure 2 shows the estimate of the Radial distribution function for the ground state of the hydrogen atom in 3 dimensions using three terms of the expansion, the exact result (obtained from [11]) is also present in the figure for comparison.

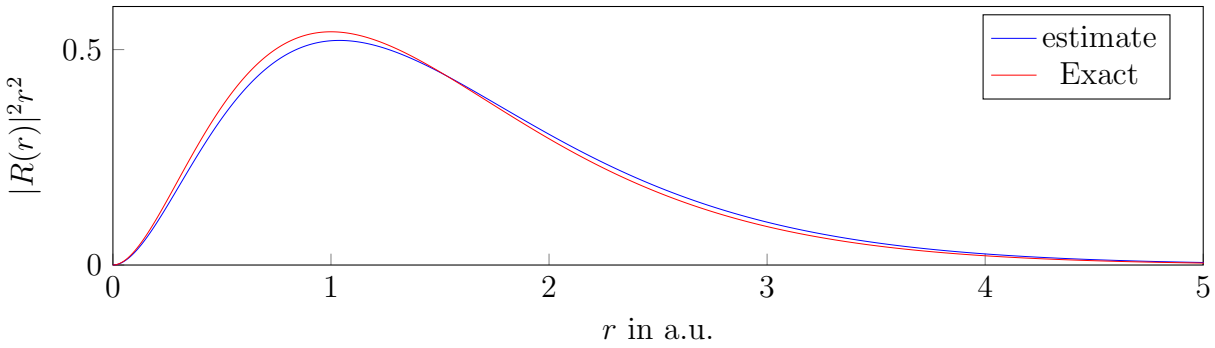

Fig. 2: The Figure shows the estimate of the radial probability density as a function of the radial distance compared to the exact known result for the ground state of the Hydrogen Atom. The estimate was constructed using only the first three terms of the $\frac{1}{N}$ expansion.

The performance of the estimate with only three terms of the series is quite remarkable as it can already capture the behaviour of the exact result. It was chosen to show the estimate including only three terms, as the difference between the estimated curve and the exact one becomes negligible once more terms are added.

2.3.2 Excited States

So far, we have only discussed the ground state of the system. However, the method discussed above can be adapted to generate an expansion for excited states. The first thing to bear in mind is that the method outlined in the section above is valid for all states with no radial nodes [7]. That means that in the case of the Hydrogen atom, this is valid for states that satisfy the equation $n - l - 1 = 0$ where n is the radial quantum number ($n = 1$ for the ground state), so it is valid for 1s, 2p, 3d...[4]

Before generalizing the method to states with j radial nodes, it is perhaps easier to look at the case of states with one radial node. In the Riccati method, we proposed $g(x) = e^{\phi(x)}$ for nodeless states, so for states with one radial node, we propose the following Ansatz

$$g(x) = (x - C)e^{\phi(x)} \tag{32}$$

Where C gives the position of the node of the state [7]. This Ansatz is now substituted int Equation 18, which gives:

$$\frac{-1}{2}(\phi''(x) + \phi'^2(x))(x - C) - \phi'(x) + (x - C)\left[k^2 V_{eff} + \left(\frac{-1}{2}k + \frac{3}{8}\right) r^{-2}(x)\right] = (x - C)\xi \tag{33}$$

All that is left now is to substitute ϕ', ξ, C by power series in $\frac{1}{k}$ in the following way:

$$\xi = \sum_{n=-1}^{\infty} E^{(n)} k^{-n} \tag{34}$$

$$\phi'(x) = \sum_{n=-1}^{\infty} \phi^{(n)}(x) k^{-n} \tag{35}$$

$$C = \sum_{n=1}^{\infty} C^{(n)} k^{-n} \tag{36}$$

Inserting this power series into Equation 33, it is possible to obtain a set of recursive relations analogous to the ones described in Equations [20-23] by matching the powers of k. Appendix A shows the relations obtained for this case.

These relations were implemented in Mathematica to obtain the coefficients of the expansion of the states with one node of the Hydrogen atom. In the case of the Hydrogen atom, those are the states that satisfy the equation $n - l - 1 = 1$, so the states 2s, 3p and so on. Figure 3 shows the Estimates on the radial distribution function for the states 2s and 3p. The exact results (obtained from [11]) are included for comparison.

[4]So far we have calculated both the Energy and the wavefunction of the 1s state, for which we took l=0, to generate a result for the next nodeless states we modify the value of l in the definition of $k = N + 2l$.

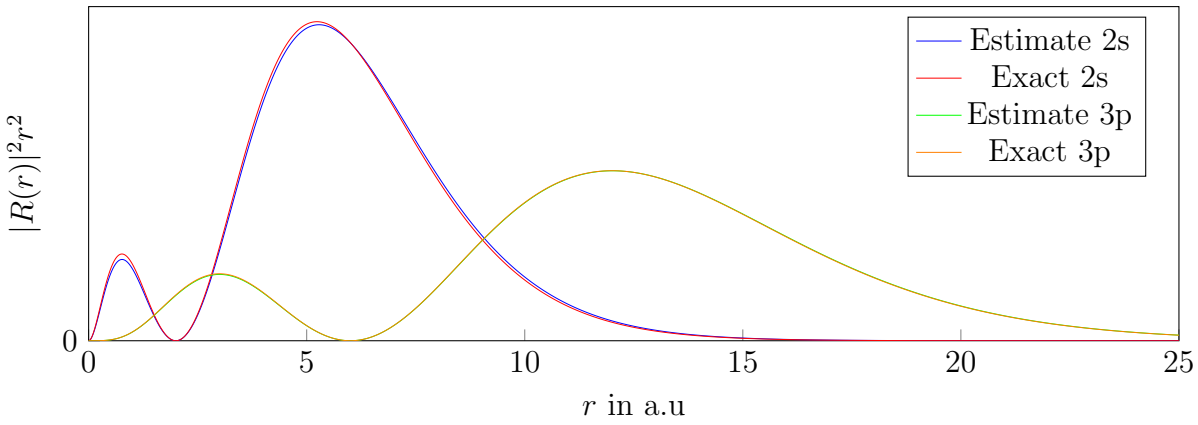

Fig. 3: The Figure shows the Estimated radial probability density as a function of the radial distance for the 2s and 3p states. The exact result for these states is also provided. The estimates were constructed using only the first four terms of the $\frac{1}{N}$ expansion. It is impossible to distinguish between the two curves using the graph.

The convergence of the method is again impressive for these states; with only four terms of the expansion, it can be seen that the estimated wavefunction of all the states can capture to correct behaviour of the exact result, including the location of the radial node. Including more terms in the expansion only improves the result.

While it is interesting to see the estimate of the wavefunctions for the excited states of the hydrogen atom, it is even more important to estimate the energy of the different excited states. The plot in figure 4 shows the partial sums $E(N)$ for different states. The states 2p contains no radial node and hence were determined using the method outlined in Section 2.3.1 and the states $2s$ and $3p$ have only one radial node, so the coefficients of the expansion were determined using the recursion relations discussed in this section.

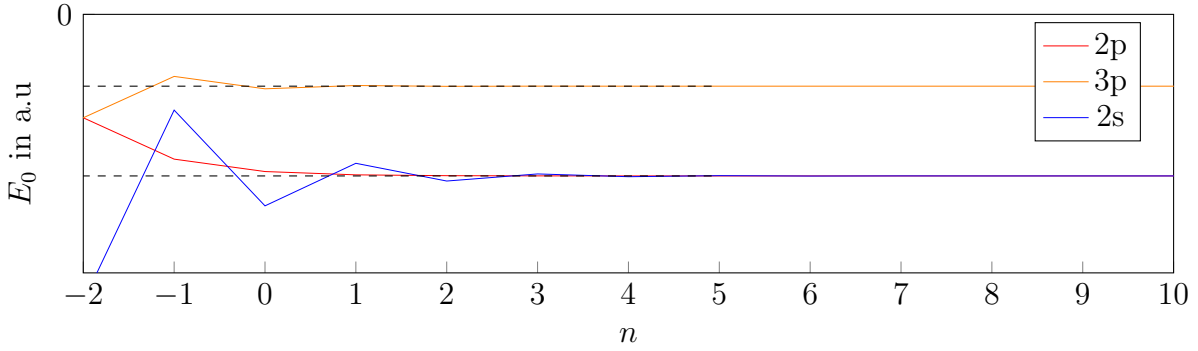

Fig. 4: Partial sums of the $\frac{1}{N}$ Expansion of the Energy of a particle in a Coulomb Potential for different bound states. A dashed line represents the exact results

The convergence of the expansion to the exact answer is, again, quite impressive for this method. Including six terms of the expansion yields a 98.8%, 99.98%, and 99.96% accuracy for the states $2s$, $2p$ and $3p$, respectively. Interestingly, this method can capture the accidental degeneracy of the states of the Hydrogen atom. The states $2s$ and $2p$ have the same energy despite the coefficients being calculated by different equations.

The only step required to generalize the method to states of j radial nodes is to modify the initial Ansatz of the wavefunction to $g(x) = \Pi_{i=0}^{j}(x - C_i)e^{\phi(x)}$ [7]. Next, this Ansatz is substituted into Equation 18. After substituting the relevant power series, the coefficients of the expansions are found by matching the different coefficients of the $\frac{1}{k}$ series and by establishing some recursion relations. While it is theoretically possible to do this for any number of radial nodes, the equations soon become intractable, and the computing power required to determine the coefficient increases rapidly.

2.3.3 Recursive Method

While the Riccati Equation method provides a systematic way of getting all the coefficients of the $\frac{1}{N}$ (or better $\frac{1}{k}$) expansion, it is not an efficient way of generating them. When it was implemented in Mathematica, getting more than a few coefficients for all but a particular class of potentials (such as the Coulomb or Yukawa Potential) was impossible. However, the Riccati method can be adapted such that the relations needed to calculate the coefficients of the Energy expansion are simplified at the cost of a loss of accuracy in the calculated wavefunction for large values of x.

As a reminder, we are trying to solve a D-dimensional problem with a potential in D dimensions that can be written as the function $V(r)$. In this case, we propose that instead, we solve a more general N-dimensional problem with potential:

$$V_N(r) = kV^*(\frac{r}{\sqrt{k}}), k = N + 2l \tag{37}$$

In which V^* is a function similar to the function V with different coupling constants such that k $V^*(\frac{r}{\sqrt{k}})$ reduces to $V(r)$ when $N = D$. For example, if we are interested in analysing $V(r) = Ar + e^{\beta r} + \frac{b}{r^2}$ in 3 dimensions (D=3), then $V^*(x) = A^*r + e^{\beta^* r} + \frac{b^*}{r^2}$, with $A^* = (3 + 2l)^{-3/2}A, \beta^* = (3 + 2l)^{1/2}\beta, b^* = (3 + 2l)^2 b$, it is easy to check that using this definition of V^*, $V_N(r)$ reduces to $V(r)$ for N=3. Again, if we can write a solution for the general problem of the N-dimensional potential, we just have to set $N = D$ at the end to get the solution for the problem that we were trying to solve:

Starting from 18, it is useful to introduce the coordinate transformation $r = \sqrt{k}\rho$, Under this transformation Equation 18 becomes:

$$\left[-\frac{1}{2k}\frac{d^2}{d\rho^2} + k\left(\frac{(1-\frac{1}{k})(3-\frac{3}{k})}{8\rho^2} + V^*(\rho)\right)\right]\gamma(\rho) = E\gamma(\rho) \tag{38}$$

$$\gamma(\rho) = u(\sqrt{k}\rho) \tag{39}$$

As before, in the large N limit, the eigenfunctions will be more and more peaked around ρ_0, which is the minimum of the leading contribution of the potential, and the Energy spectrum will tend towards [7]:

$$E_\infty = kE^{-2} = kV_{eff}(\rho_0) \tag{40}$$

$$V_{eff}(\rho) = \frac{1}{8\rho^2} + V^*(\rho) \tag{41}$$

$$\frac{d}{d\rho}\left[V_{eff}\right]_{\rho=\rho_0} = 0 \tag{42}$$

As before, for the ground state, we introduce the substitution $\gamma(\rho) = \exp\{\phi(x(\rho))\}$ with $x = \sqrt{k}(\rho - \rho_0)$ [7], which leads to the Riccati Equation:

$$\frac{-1}{2}\left[\phi''(x) + \phi'^2(x)\right] + k\bar{V}_{eff} + \left(\frac{-1}{2} + \frac{3}{8k}\right) p^{-2}(x) = \epsilon \tag{43}$$

With $\epsilon = E - kE^{(-2)}$ and $\bar{V}_{eff}(x) = V_{eff}(\rho(x)) - V_{eff}(\rho_0)$. Furthermore, we define $W(x) = k\bar{V}_{eff} + \left(\frac{-1}{2} + \frac{3}{8k}\right) p^{-2}(x)$ so that we can express the Riccati Equation on the following way:

$$\phi''(x) + \phi'^2(x) - 2W(x) + 2\epsilon = 0 \tag{44}$$

We let $y = \sqrt{k}$ and Then one substitutes the following expansions into the Riccati Equation [6]:

$$\epsilon = \sum_{n=1}^{\infty} E^{(n-1)} y^{2n} \tag{45}$$

$$\phi = \sum_{n=0}^{\infty} \sum_{m=0}^{n+1} \left(\frac{D_m^{(n)}}{2m} x^{2m} y^{2n} + \frac{C_m^{(n)}}{2m+1} x^{2m+1} y^{2n+1} \right) \tag{46}$$

$$W(x) = (W_0^{(0)} + W_2^{(0)} x^2) + (W_1^{(1)} + W_3^{(1)} x^3) y + \tag{47}$$

$$\sum_{n=2}^{\infty} \left(W_{n-2}^{(n)} x^{n-2} + W_n^{(n)} x^n + W_{n+2}^{(n)} x^{n+2} \right) y^n \tag{48}$$

The $W(x)$ coefficients are obtained by performing a Taylor expansion around $x = 0$. Once these expressions have been substituted into the Riccati equation, we match by powers of y and then by powers of x. This allows us to get a set of recursive relations for all the coefficients. These can be found in Appendix A. This method provides an easier way to calculate the coefficients of the energy expansion at the expense of accuracy in the wavefunction for large values of x [7]

3 The use of the $\frac{1}{N}$ Expansion in Quantum Mechanics

So far in this paper, the $\frac{1}{N}$ expansion has only been used for the Hydrogen atom. While this poses an excellent introductory example, it is an exactly solvable problem, so the utility of the $\frac{1}{N}$ is still unverified. This section aims to show that the $\frac{1}{N}$ expansion can be utilized to estimate with great accuracy the energy eigenvalues of different systems that do not have an exact answer. Firstly, a numerical analysis of some potential will be conducted using this method. Then a more in-depth study of the Yukawa potential will be carried out using the $\frac{1}{N}$ expansion as starting point.

3.1 Numerical Analysis of Selected Potentials

The first step towards validating the utility of the $\frac{1}{N}$ expansion technique is to estimate the energy eigenvalues of different physical systems and compare the results with the

literature values. The expansion coefficients for the different potentials were calculated using the method developed in Section 2.3.3.

The algorithm to obtain the series expansion was implemented in python. The relations of Section 2.3.3 and Appendix A were implemented in a recursive style, but memoization was used to speed up the calculations. The effect of round-off errors was analysed by comparing the Python implementation to one in Mathematica, in which all the expressions are treated symbolically. It was found that while the round-off errors start being insignificant, they become significant about the 15th order of the expansion series. Then, around the 20th order, they take over the computation, rendering the result useless. Therefore, all the results will be presented only up to the 10th order in the $\frac{1}{N}$ expansion so that the results can be completely accurate.

In many cases the $\frac{1}{N}$ expansion gives an asymptotic representation of the Energy. In general, this means that when adding the terms of the series, the partial sums converge to the correct result up to a given term, where they drift away from this result. It was found that ten terms of the series give a good convergence for the investigated potentials.

All the code developed for this project (In python and Mathematica) can be found on the Github repository of the project [12]

3.1.1 The Laser Dressed Coulomb Potential

The Time-dependent Schrodinger Equation for a hydrogen atom in an electromagnetic field is given by:

$$i\hbar\partial_t\Psi(\underline{r},t) = \left[\frac{1}{2m}\left(\hat{p}+\frac{e}{c}\underline{A}(t)\right)^2 - \frac{e^2}{r}\right]\Psi(\underline{r},t) \tag{49}$$

For the case of an intense monochromatic laser, the vector potential is described by: $\underline{A}(t) = A(\hat{x}\cos(wt)+\hat{y}\sin(wt))$ [13]. The Schrodinger Equation can be changed into a more suitable form by including the definition of $\underline{\lambda}$ [13].

$$i\hbar\partial_t\Psi(\underline{r},t) = \left[\frac{1}{2m}\hat{p}^2 - \frac{e^2}{|\underline{r}-\underline{\lambda}|}\right]\Psi(\underline{r},t) \tag{50}$$

$$\underline{\lambda}(t) = -\frac{e}{mc}\int^t dt'\underline{A}(t') \tag{51}$$

This potential can now be expanded as:

$$V(\underline{r}) \approx \frac{-e^2}{\sqrt{r^2+\lambda^2}}\left(1-\frac{\underline{r}\cdot\underline{\lambda}}{r^2+\lambda^2}+...\right) \tag{52}$$

With $\lambda = |\underline{\lambda}| = \frac{Ae}{wmc}$ (time independent). It has been shown in [14] that this series converges rapidly and that, therefore, it is reasonable to approximate the potential by retaining only the leading term,$V(r) = \frac{-e^2}{\sqrt{r^2+\lambda^2}}$ [15; 13], in which λ is related to the intensity ($I(\frac{W}{cm^2})$) and frequency ($\omega(s^{-1})$) of the Laser by the equation $\lambda = 6.5\times10^{24}w^{-2}\sqrt{I}$ [15]. This potential can now be treated as an approximate stationary potential that describes the energy levels of the hydrogen atom in the electromagnetic wave field [15; 13].

Therefore, we will now explore the Energy levels of this system for different values of λ using the $\frac{1}{N}$ expansion. A portion of the obtained results is shown in Table 1

	E in atomic units ($m = \hbar = e = 1$)			
λ	1s	2s	2p	3p
1	-0.275748	0.098219	-0.113078	-0.052024
Numerical [15]	-0.274891	-0.092679	-0.113024	-0.052060
5	-0.107130	-0.053026	-0.068179	-0.037366
Numerical [15]	-0.107081	-0.053171	-0.068187	-0.037361
10	-0.063738	-0.037157	-0.046199	-0.028313
Numerical [15]	-0.063739	-0.037154	-0.046199	-0.028314

Table 1: Estimate of the energy of different states of the system described by the potential $V(r) = -\frac{e^2}{\sqrt{r^2+\lambda^2}}$ for two different values of λ using the $\frac{1}{N}$ expansion. The numerical results are provided for comparison with the estimates

It can be seen that the convergence of the first ten terms of the $\frac{1}{N}$ series is good for all the values of λ used. It was found that the convergence of the method improves when increasing the value of λ and that for a given value of λ, it worsens for states with more nodes in the radial wavefunction (higher excited states). This is a general behaviour we observe when using the $\frac{1}{N}$ expansion [5]. Additionally, from the results of Table 1, it can be deduced that one of the effects that the electromagnetic field has on the energy levels is that it removes the accidental degeneracy present in the Hydrogen atom, now two states with the same value of the radial quantum number but different l do not have the same energy.

3.1.2 The Spiked Harmonic Oscillator

The spiked harmonic oscillators potentials refer to a class of potentials described by the equation:

$$V(r) = r^2 + \frac{\lambda}{r^\alpha} \tag{53}$$

λ is a positive coupling constant, and α is a positive constant determining the type of singularity on the origin [16]. One of the interesting properties of this potential is that the coulomb-like term $\frac{\lambda}{r}$ creates an infinite potential barrier at the origin, which means that this term cannot be neglected even for small values of λ. On the other hand, it is not possible to neglect the first term of the interaction when $\lambda \to \infty$ because it is responsible for the existence of bounded states.

Additionally, there are two different regions of for α. For $\alpha < \frac{5}{2}$, the ground state has a perturbation series in powers of λ but in the region $\alpha \geq \frac{5}{2}$ (supersingular region) standard perturbation theory fails [17]. Therefore, we will now use the $\frac{1}{N}$ expansion to

obtain values for the energy of the ground state of this system for the case $\alpha = \frac{5}{2}$ which is in the supersingular region and the simple case of $\alpha = 1$

The results for the Ground state energy of the system with $\alpha = \frac{5}{2}$ and for different values of the coupling constant are shown below in table 2.

	E of the Ground State in atomic units ($2m = \hbar = 1$)		
λ	$\frac{1}{N}$	Numerical [18]	Error (%)
0.01	3.0331630	3.036729	0.12
0.1	3.2688843	3.266873	0.06
1.0	4.3161857	4.317311	0.03
10	7.7351097	7.735111	1.68×10^{-5}
100	17.5418902	17.541889	6.84×10^{-6}
1000	44.9554848	44.955485	4.45×10^{-7}

Table 2: Estimate of the energy of the ground state of the system described by the potential $V(r) = r^2 + \frac{\lambda}{r^{5/2}}$ for different values of λ using the $\frac{1}{N}$ expansion. The numerical results are provided for comparison with the estimates

The results obtained with our method for the $\alpha = \frac{5}{2}$ are in good agreement with values obtained by numerically integrating the Schrodinger Equation. It was also found that the convergence of our results improves in the region where the coupling constant is large.

On the other hand, The results obtained for the case of the charged harmonic oscillator and different values of λ are presented below in table 3,

	E of the Ground State in atomic units ($2m = \hbar = 1$)		
λ	$\frac{1}{N}$	Exact [17]	Error (%)
0.01	3.01127608	3.01127601	2.32×10^{-6}
1.00	4.05787497	4.05787701	5.03×10^{-5}
10.0	10.5774667	10.5774834	1.58×10^{-4}

Table 3: Estimate of the energy of the ground state of the system described by the potential $V(r) = r^2 + \frac{\lambda}{r}$ for different values of λ using the $\frac{1}{N}$ expansion. The numerical results are provided for comparison with the estimates

The convergence of the $\frac{1}{N}$ expansion retaining ten terms was extremely successful. The results show that the opposite behaviour as in the case of $\alpha = \frac{5}{2}$ as the convergence is better for small values of the coupling constant.

3.2 The Yukawa Potential

The following equation describes the Yukawa potential:

$$V_{\text{Yukawa}} = -a\frac{e^{-\lambda r}}{r} \tag{54}$$

This potential tends to the Coulomb-like potential ($\frac{-a}{r}$) in the limit $r \to 0$, and it is exponentially damped for large values of r. It belongs to the class of Coulomb-screened potentials, and it has a variety of applications in different branches of physics (see References [19; 20] as examples). Additionally, it has the interesting property of having both bounded and scattering states [21].

Given that there is no exact answer to the Schrodinger equation for this potential, several methods have been employed in the past to study them, including the $\frac{1}{N}$ expansion. This section explains how the above methods can be adapted to study this system in great detail (The method was initially proposed in [8]) and provides some of the results obtained while studying them.

3.2.1 Adapting the Riccati Equation Method

It is possible to slightly adapt the Riccati Equation method developed in section 2.3.1 to obtain the coefficients of the $\frac{1}{N}$ expansion in the case of the Yukawa potential up to very high orders, we will now exemplify it with the Ground State (states with no nodes). However, it can be generalized to excited states. Therefore, the first step in the method is to define $V_N(r)$. In this case, we chose to define it as [22]:

$$V_N(r) = -\frac{ak^2 e^{\left(\frac{-(D+2l)^2\lambda r}{k^2}\right)}}{(D+2l)^2 r} \tag{55}$$

This potential reduces to the usual Yukawa potential when we set $N = D$. We are interested only in the 3-dimensional case, so we can directly substitute $D = 3$. The advantage of this choice of potential is that the exponential factor goes to 1 in the large k limit. We now proceed as usual by defining

$$\bar{V}(r) = -\frac{\bar{a}e^{\left(\frac{-(3+2l)^2\lambda r}{k^2}\right)}}{r} \tag{56}$$

With $\bar{a} = \frac{a}{(3+2l)^2}$. This can now be substituted into Equation 20. As before, we define the effective potential in the large k limit, giving $V_{eff}(r) = \frac{1}{8r^2} - \frac{\bar{a}}{r}$ (the exponential term goes to 1 in the large k limit) and as usual $E_\infty = k^2 V_{eff}(r_0) = k^2 E^{(-2)}$, with r_0 being the minimum of the effective potential. Therefore, $E^{(-2)} = -2\bar{a}$.

To obtain the other coefficients of the series, we make the usual change $x = r - r_0$, and we make the Ansatz $u(x) = e^{\phi(x)}$ which leads to:

$$\frac{-1}{2}\left[\phi'(x)^2 + \phi''(x)\right] + k^2\bar{V}_{eff} + \left(\frac{3}{8} - \frac{k}{2r^2(x)}\right)r^{-2}(x) + k^2\sum_{k=1}^{\infty}\frac{(-1)^{n+1}\bar{a}(\lambda(3+2l)^2)^n}{k^{2n}n!} = \xi \tag{57}$$

And as before, $\bar{V}_{eff} = V_{eff} - V_{eff}(r_0)$ and $\xi_0 = E - k^2 V_{eff}(r_0)$. This is similar to 23 with an additional term that comes from Taylor expanding the exponential in powers of $\frac{1}{k}$. Now we make the same substitutions as before:

$$\xi = \sum_{n=-1}^{\infty} E^{(n)} k^{-n} \qquad\qquad \phi'(x) = \sum_{n=-1}^{\infty} \phi^{(n)}(x) k^{-n} \tag{58}$$

And we match the powers of k to obtain a set of recursive relations that will allow us to obtain the coefficients.

This method works for states with no radial nodes, that is, states that satisfy $n-l-1=0$ [22] where n is the radial quantum number (we expect this system to behave similarly to the case of the Coulomb potential [22]). To generalize the method for states with i radial nodes (those that satisfy the equation $n-l-1=i$), we modify the Ansatz to:

$$u(x) = \Pi_{j=1}^{i}(x - C_j)e^{\phi(x)} \tag{59}$$

And we expand each C_j as a power series on k, $C_j = \sum_{n=1}^{\infty} C_j^{(n)} k^{-n}$. Doing this is now possible to find a set of recursive relations for the coefficients of these states too [22].

3.2.2 Summing the $\frac{1}{N}$ expansion

This method has been implemented in Mathematica, and an analytic expression has been found for the coefficients of the $\frac{1}{N}$ expansion up to very high order (it was possible to calculate around ≈ 200 terms of the expansion for both potentials in reasonable computation time for different states). Once the coefficients have been found, it is time to extract information from the series. However, suppose we try to directly calculate the partial sums up to high order for $N = 3$ and for different values of the coupling parameter a and screening parameter λ. In that case, we will get a non-sensible answer for the Energy for most values of a, λ. This is a consequence of the $\frac{1}{N}$ expansion being a divergent series and an asymptotic representation of the energy, which implies that naively adding up the terms will not often work when high-order terms of the series are included [6].

While it might appear that we are gaining no information out of calculating high-order terms of the series, it is usually the case that a lot can be extracted from divergent series. For this particular case, two methods were tried to extract information directly from the $\frac{1}{N}$ expansion (A Padé Approximation of the series and a Padé-Borel summation), and they both failed. Therefore, an alternative approach was used. Following [8], it was found that we can restructure the $\frac{1}{N}$ series as a perturbation series of the parameter $\beta = \frac{\lambda}{a}$ that is to say:

$$\sum_{n=-2}^{\infty} E^{(n)} k^{-n} \to a^2 \sum_{n=0}^{\infty} a_n(k) \beta^n \tag{60}$$

Restructuring the partial sums in powers of β instead of in powers of k makes it possible to obtain the coefficients that one would obtain using standard perturbation theory [8]. Therefore, it is possible to obtain the coefficients of the traditional perturbation series using the $\frac{1}{N}$ series. However, it must be noted that there is not a 1-1 correspondence

between the two series. That is to say, calculating the first i coefficients of the $\frac{1}{N}$ expansion will not suffice to obtain the first i coefficients of the perturbation series.

The first coefficient of the perturbation series, $a_0(k)$, corresponds to the case $\beta = 0$. Therefore we know that it will be equal to the $\frac{1}{N}$ expansion of the hydrogen atom [8], which means that it involves an infinite number of coefficients of the $\frac{1}{N}$ expansion. However, we already know that the expansion converges to the known exact solution in the case of the Hydrogen atom [5], so the first coefficient $a_0(k)$ can be calculated without the need to calculate an infinite number of coefficients[5]. Subsequent terms in the perturbation series do not involve infinite coefficients of the $\frac{1}{N}$, but we must be careful when moving from one series to the other.

For example, if we calculate the partial sum including the first 13 terms of the $\frac{1}{N}$ expansion (of the states with no radial nodes) and we restructure the result as a series of β we obtain:

$$a^2\left(a_0+\beta+\left(\frac{(3+2l)^4}{8k^3}-\frac{(3+2l)^4}{8k^2}\right)\beta^2+\left(\frac{1}{k^7}-\frac{1}{k^6}-\frac{1}{k^5}+\frac{1}{k^4}\right)\frac{(3+2l)^8}{96}\beta^3+O(\beta^4)\right) \tag{61}$$

While higher powers than β^3 are found when restructuring the partial sum, these do not match the perturbation series' coefficients. This occurs because those terms depend on higher order coefficients of the $\frac{1}{N}$. It is possible to check up to what order of perturbation series the partial sum of the $\frac{1}{N}$ expansion series up to order i provides by comparing the series on β that you obtain in using the partial sums of the $\frac{1}{N}$ expansion up to order i and $i+1$.

At first hand, it might appear that we have accomplished nothing. We still cannot try to directly sum the series for most of the values of β. However, It has been shown that a Padé Summation of this series can be used to obtain accurate results[6] [4; 21]. Therefore, taking a slight detour makes it possible to extract useful information from the coefficients calculated in the method outlined in the previous section.

3.2.3 Analysis and Results

Using the coefficients of the $\frac{1}{N}$ expansion to calculate the coefficients of the perturbation series and making a Pade approximation of the perturbative series, the energy eigenvalues of the system described by the Yukawa potential were estimated to great accuracy for different values of the screening parameter. Without any loss of generality, we set $a = 1$ to compare our results with the literature, so $\beta = \lambda$.

The values of the Energy (in atomic units) for different states and values of λ are shown in Table 4. The values of Reference [24] are provided for comparison.

[5]Using our formulation the first coefficient is $a_0 = \frac{-2k^4}{(k-1)^2(3+2l)^4}$ for states with no nodes

[6]It is vital to bear in mind that we have not shown that the perturbation series of this system has a zero radius of convergence, we have just noted that the perturbation series seems to diverge for most the values of β. Even if the series has a small radius of convergence β^* (which seems unlikely), we can use the Padé summation method to obtain accurate results outside of the region of convergence of the perturbation series [23].

	E in atomic units ($m = \hbar = 1$)			
	$1s$		$2p$	
λ	$\frac{1}{N}$	Ref [24]	$\frac{1}{N}$	Ref [24]
0.01	-0.490075	-0.49005	-0.115245	-0.11525
0.02	-0.480296	-0.48030	-0.105963	-0.10596
0.05	-0.451816	-0.45180	-0.0807404	-0.08074
0.1	-0.407058	-0.40706	-0.0465344	-0.04654
0.2	-0.326809	-0.32681	-0.00410068	-0.00410
0.5	-0.148117	-0.14812	-	-
1.15	-0.0004559	-0.00046	-	-
	$2s$		$3p$	
λ	$\frac{1}{N}$	Ref [24]	$\frac{1}{N}$	Ref [24]
0.005	-0.120074 5	-0.12005	-0.0507082	-0.05070
0.01	-0.115293	-0.11529	-0.0461531	-0.04616
0.02	-0.106148	-0.10615	-0.0378524	-0.03785
0.05	-0.0817712	-0.08177	-0.0185578	-0.01856
0.1	-0.0499283	-0.04993	-0.00158867	-0.00159
0.2	-0.0121079	-0.01211	-	-
0.3	-0.000091	-0.00009	-	-

Table 4: Estimate of the energy of different states of the system described by the potential $V(r) = -\frac{e^{-\lambda r}}{r}$ for different values of λ. The values were calculated by making a Padé with the first 25 coefficients in perturbation theory (Obtained through the $\frac{1}{N}$ expansion).

The accuracy of our method's results is impressive in all cases. One of the peculiarities of the Yukawa potential is that it has both bound and scattering states [21]. Each state has a value of λ, often called λ^*, for which that bound state ceases to exist (the energy goes to the continuum) [21]. In Table 4, the energies of the different states have been presented up to the approximate value of λ^* for each state. An important feature of our analysis is that it gives good results for all the range $0 \leq \lambda \leq \lambda^*$ for the different states.

Furthermore, It is possible to use this method to try and estimate the value of lambda (λ_{crit}) for which no bound states exist, that is, the λ^* of the ground state. If we plot our values for the energy for the ground state for larger values of λ than the ones presented in Table 4, we find that it starts in the Coulomb value and it tends towards $E \approx 0$ (Which would happen at $\lambda = \lambda_{\text{crit}}$ but then they reach a maximum and they start decreasing monotonically. The region in which it starts decreasing monotonically corresponds to the unphysical region of $\lambda \geq \lambda_{\text{crit}}$ for which the bound state does not longer exist (and

therefore, our analysis is not valid in that region). The graph of the ground state Energy as a function of λ is shown in Figure 5.

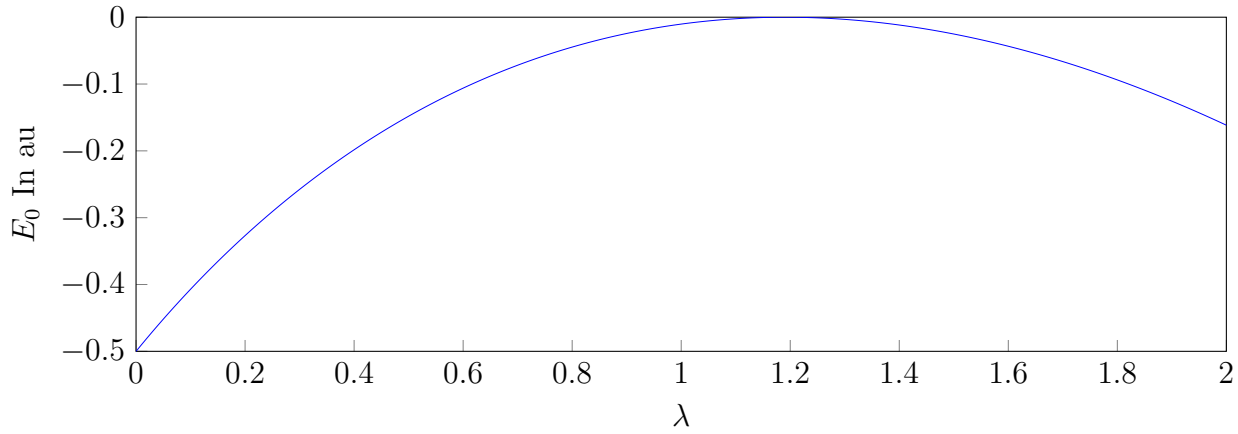

Fig. 5: Padé of the Perturbation Series of the ground state energy including 50 terms for different values of λ, including values larger than the estimated critical parameter.

Hence, it is possible to find an approximate value of the parameter λ_{crit} by numerically determining the maximum of the Energy $-$ λ graph. The value of λ_{crit} found using this method was $\lambda_{\text{crit}} = 1.19061$, which is extremely close to the accurate value of $\lambda_{\text{crit}} = 1.1906122105(5)$ found in Reference [25].

Another important feature of this system is that the exponential factor has the effect of lifting the accidental degeneracy on the energy levels that was present in the case of the Hydrogen atom, as in the case of the Laser Dressed Coulomb Potential, two levels with the same radial quantum number but different l now do not have the same eigenvalue. It is interesting to see how that difference evolves as a function of the screening parameter. For that purpose, Figure 6 shows the Energy curves of the states 2s and 2p for different values of λ, and each of the graphs is plotted up to the λ^* for each state.

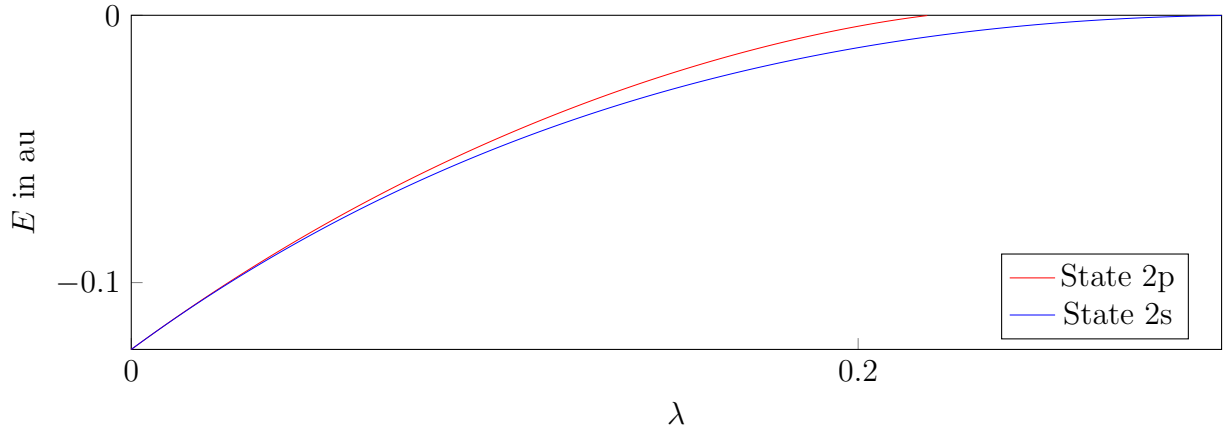

Fig. 6: Energy curves obtained for different values of the screening parameter for the states 2s and 2p of the system with a Yukawa potential

As expected, in the limit $\lambda \to 0$, the two Energy curves meet as the potential reduces

to the usual Coulomb potential and the degeneracy is recovered. In general, it is seen that the difference between the levels increases with the value of the screening parameter. Regarding ordering energy levels, for a given value of n, the energy increases with l. While this was only numerically confirmed for the limited set of investigated states (1s,2s,2p,3p,3d), Reference [15] confirms this behaviour is indeed characteristic of the Yukawa potential and true for all the states.

Finally, analysing the improvement gained by transforming the $\frac{1}{N}$ expansion to a traditional perturbation series and performing a Padé on it is interesting. The plot on Figure 7 shows the Energy $-\lambda$ graph generated using the Perturbation Series (blue) and the graph generated by using the first five coefficients of the $\frac{1}{N}$ expansion[7] for the case of the Ground State.

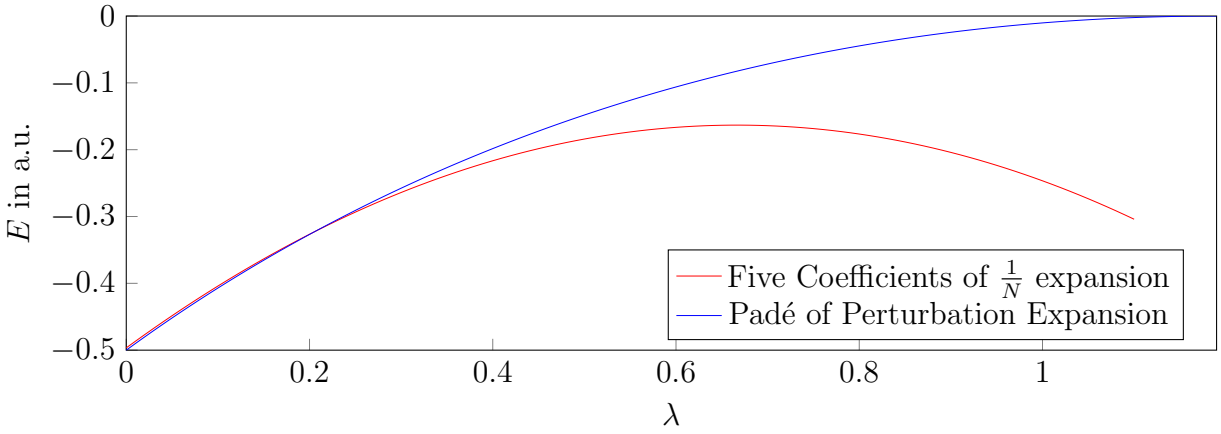

Fig. 7: The Figure shows the Energy curves of the ground state as a function of λ that are obtained through the Padé Summation of the perturbation series (blue) and the direct evaluation of the first five terms of the $\frac{1}{N}$ expansion (red)

Given that the values of the perturbation series are extremely accurate for the region $0 \leq \lambda \leq \lambda_{\text{crit}}$ it can be used as a measure of accuracy when comparing it to the values given by the red curve. While using the directly the $\frac{1}{N}$ expansion yields decent results in the region $\lambda < 0.3$, in the region $0.3 \leq \lambda \leq \lambda_{\text{crit}}$ it is not able to capture the correct behaviour of the ground state Energy. Therefore, it is evident that transforming the $\frac{1}{N}$ expansion to the perturbative series has allowed us to extend the domain in which our analysis is accurate.

While for the purpose of the report, only the Yukawa potential was analysed using this method up to high order, it is also possible to slightly adapt it to study the Expontentially Cosine Screened Coulom (ECSC) up to very high order. Reference [22] outlines the method in this case and works out the first orders.

[7]This number of coefficients was used as it gave a good convergence for the largest region of λ

4 Conclusion and Further Work

The numerical results obtained in Section 3 show that using a small number of terms of the $\frac{1}{N}$ expansion yield a good description of the Energy eigenvalues of different physical systems for low-lying states. Furthermore, the expansion coefficients can be obtained using a simple set (in the case of low-lying states) of recursion relations that can be easily implemented in any computer language, and the computing power required to generate the first coefficients is negligible (none of the computations took more than 10 seconds to run). The combination of the method's accuracy with a few coefficients and the fact that they can be easily calculated makes this method powerful for obtaining high-quality estimates of the Energy eigenvalues of the Schrodinger equation for different potentials. Given that this method gives remarkably accurate results for low-lying states, it can be combined with WKB methods which are more accurate for highly excited states [26].

Additionally, this paper has also shown an example in which the expansion coefficients up to high order (around 200) were calculated and used to analyse with great detail the system described by the Yukawa potential.

Despite the evident success of the techniques explained in this paper, it is important to mention some of the shortcomings of the methods used and of the $\frac{1}{N}$ expansion as a whole. This also provides an excellent opportunity to discuss possible options for further work on the project.

Firstly, the method used to determine the series coefficients becomes almost intractable in the case of states with more than two radial nodes. It becomes increasingly hard to obtain a set of recursive relations. And even if these are found, they become more complicated (which would increase the computational time required to get the coefficients). A possible way around this problem is to look at other methods for generating the $\frac{1}{N}$ expansion. A natural continuation of the project would be to look into the Hypervirial method for generating this expansion. Reference [5] describes alternative several methods of obtaining the series, and the Hypervirial method to obtain the $\frac{1}{N}$ expansion for the case of the ECSC potential is used in [27].

Secondly, the series can have slow convergence and worsens in the case of excited states. This issue can be solved by using the Shifted $\frac{1}{N}$ expansion instead of the regular $\frac{1}{N}$. In the Shifted $\frac{1}{N}$ series, the expansion parameter is no longer k but $\bar{k} = k - a$, where a is a parameter that is determined on physical grounds and has the effect of accelerating the convergence of the series. This new parameter generally depends on the radial quantum number, so it improves the convergence for excited states. An introduction to this method can be found on [28] and References [15] and [16] apply in the case of the Laser Dressed Coulomb Potential and the Spiked Harmonic Oscillator respectively.

Finally, the method used to obtain information from the divergent $\frac{1}{N}$ series in the case of the Yukawa potential requires an intermediate step of restructuring the partial sums as a traditional perturbation series. It was impossible to extract the information directly from the coefficients of the original expansion despite using two different methods (Padé Summation and Borel-Padé Summation). Therefore, it would be interesting to try and investigate further why this is happening and whether other methods might be applicable in this case. The first step towards this goal would probably be estimating the asymptotic

growth of the $\frac{1}{N}$ expansion coefficients.

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A Appendix One: Mathematical Relations

Recursive Relations for states with two Radial nodes (Riccati Method) [5]

$$\phi^{(-1)}(x) = -\sqrt{2V_{eff}(x)} \tag{62}$$

$$x\sqrt{2V_{eff}(x)}\phi^{(0)}(x) = x\left[E^{(-1)} + \frac{1}{2}\phi^{(-1)\prime}(x) + \frac{1}{2}r^{-2}(x)\right] + \phi^{(-1)}(x) \tag{63}$$

$$x\sqrt{2V_{eff}(x)}\phi^{(1)}(x) = x\left[E^{(0)} + \frac{1}{2}\phi^{(0)\prime}(x) + \frac{1}{2}(\phi^{(0)2}) - \frac{3}{8}r^{-2}(x)\right] - \tag{64}$$

$$C^{(1)}\left[E^{(-1)} + \frac{1}{2}\phi^{(-1)\prime}(x) + \phi^{(-1)}(x)\phi^{(0)}(x) + \frac{1}{2}r^{-2}(x)\right] + \phi^{(0)}(x) \tag{65}$$

$$x\sqrt{2V_{eff}(x)}\phi^{(2)}(x) = x\left[E^{(1)} + \frac{1}{2}\phi^{(1)\prime}(x) + \phi^{(0)}\phi^{(1)}\right] - \tag{66}$$

$$C^{(1)}\left[E^{(0)} + \frac{1}{2}\phi^{(0)\prime}(x) + \phi^{(1)}(x)\phi^{(-1)}(x) + \frac{1}{2}(\phi^{(0)2}) - \frac{3}{8}r^{-2}(x)\right] - \tag{67}$$

$$C^{(2)}\left[E^{(-1)} + \frac{1}{2}\phi^{(-1)\prime}(x) + \phi^{(-1)}(x)\phi^{(0)}(x) + \frac{1}{2}r^{-2}(x)\right] + \phi^{(1)}(x) \tag{68}$$

$$x\sqrt{2V_{eff}(x)}\phi^{(n)}(x) = x(E^{(n-1)} + \frac{1}{2}\phi^{(n-1)\prime}(x) + \frac{1}{2}\sum_{m=0}^{n-1}\phi^{(m)}(x)\phi^{(n-m-1)}(x)) - \tag{69}$$

$$\sum_{m=1}^{n-2}C^{(m)}(E^{(n-m-1)} + \frac{1}{2}\phi^{(n-m-1)\prime}(x) + \frac{1}{2}\sum_{p=-1}^{n-m}\phi^{(p)}(x)\phi^{(n-m-p-1)}(x)) - \tag{70}$$

$$C^{(n-1)}\left(E^{(0)} + \frac{1}{2}\phi^{(0)\prime}(x) + \phi^{(1)}(x)\phi^{(-1)}(x) + \frac{1}{2}(\phi^{(0)2}) - \frac{3}{8}r^{-2}(x)\right) - \tag{71}$$

$$C^{(n)}\left[E^{(-1)} + \frac{1}{2}\phi^{(-1)\prime}(x) + \phi^{(-1)}(x)\phi^{(0)}(x) + \frac{1}{2}r^{-2}(x)\right] + \tag{72}$$

$$\phi^{(n-1)}(x), n > 2 \tag{73}$$

It is not hard to see that the equations are more complicated than the ones obtained for the nodeless states. Furthermore, extracting the different coefficients from these equations is also a harder process. One starts by obtaining an expression for $\phi^{(-1)}$ using the same relation as we used before, then we differentiate the next equation, and we evaluate it at $x = 0$ to obtain an expression for $E^{(-1)}$. Using the same equation now that we know all the coefficients at the right-hand side, we can get an expression for $\phi^{(0)}$. In the third equation we start by evaluating it at $x = 0$, which gives $C^{(1)}$ and then we repeat the process of differentiating to obtain $E^{(0)}$ and then we obtain $\phi^{(1)}$. This process can be repeated to obtain the necessary coefficients of the expansion.

Recursive Relations for states with one Radial node (Recursive Method) [6]

$$C_m^{(n)} = -\frac{1}{2D_1^{(0)}}\left(-2W_{2m+1}^{(2n+1)} + 2(m+1)C_{m+1}^{(n)} + 2\sum_{i=1}^{n}\sum_{j=1}^{i+1} D_j^{(i)} C_{m+1-j}^{(n-i)}\right) \tag{74}$$

$$D_m^{(n)} = -\frac{1}{2D_1^{(0)}}\left(-2W_{2m}^{(2n)} + (2m+1)D_{m+1}^{(n)} + \sum_{i=1}^{n-1}\sum_{j=1}^{i+1} D_j^{(i)} D_{m+1-j}^{(n-i)} + \sum_{i=0}^{n-1}\sum_{j=0}^{i+1} C_j^{(i)} C_{m-j}^{(n-i-1)}\right) \tag{75}$$

$$E^{(n-1)} = \frac{1}{2}\left(-D_1^{(n)} + 2W_0^{(2n)} - \sum_{i=0}^{n-1} C_0^{(i)} C_0^{(n-i-1)}\right) \tag{76}$$

With $D_1^{(0)} = -\sqrt{2W_2^{(0)}}$, $D_{n+2}^{(n)} = C_{n+2}^{(n)} = 0$ and $D_m^{(n)} = C_m^{(n)} = 0$ if $m < 0$ (also $D_0^{(n)} = 0$).

Recursive Relations for states with two Radial nodes (Recursive Method) [6]

$$T_m^{(n)} = \sum_{k=1}^{n-m} a_k S_m^{(n-k)} - 2D_{m+1}^{(n)} \tag{77}$$

$$S_m^{(n)} = \sum_{k=1}^{n-m} a_k T_{m+1}^{(n-k+1)} - 2C_{m+1}^{(n)} \tag{78}$$

$$a_n = \frac{1}{T^{(0)}{}_0}\left(2C_0^{(m-1)} - \sum_{k=1}^{n-1} a_k T_0^{(n-k)}\right) \tag{79}$$

$$C_m^{(n)} = -\frac{1}{2D_1^{(0)}}\left(-S_m^{(n)} - 2W_{2m+1}^{(2n+1)} + 2(m+1)C_{m+1}^{(n)} + 2\sum_{i=1}^{n}\sum_{j=1}^{i+1} D_j^{(i)} C_{m+1-j}^{(n-i)}\right) \tag{80}$$

$$D_m^{(n)} = -\frac{1}{2D_1^{(0)}}\left(-2W_{2m}^{(2n)} + (2m+1)D_{m+1}^{(n)} + \sum_{i=1}^{n-1}\sum_{j=1}^{i+1} D_j^{(i)} D_{m+1-j}^{(n-i)} + \sum_{i=0}^{n-1}\sum_{j=0}^{i+1} C_j^{(i)} C_{m-j}^{(n-i-1)}\right) \tag{81}$$

$$E^{(n-1)} = \frac{1}{2}\left(T_0^{(m)} - D_1^{(n)} + 2W_0^{(2n)} - \sum_{i=0}^{n-1} C_0^{(i)} C_0^{(n-i-1)}\right) \tag{82}$$

With $D_1^{(0)} = -\sqrt{2W_2^{(0)}}$, $D_{n+2}^{(n)} = C_{n+2}^{(n)} = 0$ and $D_m^{(n)} = C_m^{(n)} = 0$ if $m < 0$ (also $D_0^{(n)} = 0$). To obtain this recursion relations we make the Ansatz $\gamma(\rho) = (xy - A(y))e^{\phi(x(\rho))}$ and we expand $A(y) = \sum_{n=1}^{\infty} a_n y^{2n}$.