Padé and Algebraic Approximants applied to the Quantum Anharmonic Oscillator

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Abstract: The Hypervirial and Hellmann-Feynman Theorems are applied to the quantum anharmonic oscillator to find recurrence relations for the coefficients of the expansion of the energy. Padé and Algebraic Approximants are used to assign a sum to the resulting divergent series and are discussed in comparison with the Taylor Series Expansion of a known function. In the future, the results from the quantum anharmonic oscillator will be compared to those that arise from different methods of assigning sums such as the Borel Method of Resummation and the Aitken's Delta-Squared Method.

1. INTRODUCTION

Motivation. It is well known in quantum mechanics that the Schrödinger equation cannot be solved except for some simple models. Yet, the Schrödinger equation is used to describe many quantum mechanical systems. One of the main ideas in quantum mechanics is to solve the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2}+\frac{1}{2}m\omega^2x^2\Psi(x)=E\Psi(x)$$

for the wavefunction, $\Psi(x)$, and the energy, E. The Schrödinger equation is simply a second order variable coefficient linear differential equation that can be solved exactly by "brute force" using the method of power series expansion from differential equations or by using ladder operators from quantum mechanics. However, the anharmonic oscillator cannot be solved exactly and some of the ideas of quantum mechanical perturbation theory must be used.

The Schrödinger equation for the anharmonic oscillator discussed in this paper is:

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2}+\left(\frac{1}{2}\omega^2x^2+\frac{1}{2}\lambda x^2+\lambda^2x^3\right)\Psi(x)=E\Psi(x).$$

To solve this equation we must first use the Hypervirial and Hellmann-Feynman Theorems coupled with multiple commutator relations to expand the equation. Once the Schrödinger equation is expanded we can assume a power series expansion for the energy, collect like powers of λ (the perturbation parameter) and set their coefficients equal to 0. Once this is done it becomes possible to calculate the coefficients in the expansion of the energy; a divergent series.

This paper is organized as follows. In Section 2 we review some ideas of power series and Taylor series expansions. Padé approximants are then introduced in Section 3 as a generalization of the Taylor polynomials and then extended to Algebraic approximnats. In Sections 4 and 5 the Schrödinger equation for the quantum anharmonic oscillator is solved for the energy using the Hypervirial and Hellmann-Feynman Theorems (the details are left as appendices). Resulting in an infinite power series expansion of the energy in the perturbation parameter. The coefficients in the resulting series are then used to initialize both the Padé and Algebraic approximants and the energy for the quantum anharmonic oscillator is calculated in Section 6.

2. SERIES, POWER SERIES, RADIUS OF CONVERGENCE, AND TAYLOR SERIES EXPANSIONS

Series. A series is an infinite ordered set of terms combined together by addition operators (i.e. + and -). A series can be either finite or infinite and sometimes the term infinite series is used to emphasize the fact that series contain an infinite number of terms. An example might be $1+1+2+3+5+8+\ldots$. An infinite series is usually denoted $\sum_{n=0}^{\infty} a_n$ or $\sum a_n$. The sum of an infinite series is a limit of the partial sums of finitely many terms $(i.e.\ \lim_{N\to\infty}\sum_{n=0}^{N} a_n)$ where the elements, a_n, are either real or complex numbers, provided such a limit exists. If such a limit has a finite value, the series is said to converge, if it does not, the series is divergent. If this limit exists and is equal to s, for example, then it is said that the series converges toward s. Simply stated, a series converges if the sequence of partial sums has limit s, as $N \to \infty$.

A general definition from calculus is that for a given series $\sum_{n=1}^{\infty} a_n = a_1 + a_2 + a_3 + \cdots$, if s_N denotes the Nth partial sum:

$$s_N = \sum_{i=1}^{N} a_i = a_1 + a_2 + \cdots + a_n$$

If the $\lim_{N\to\infty} s_N = s$ exists the series is said to be convergent and thus

$$\sum_{i=1}^{\infty} a_i = s$$

where the number s is called the sum of the series. Otherwise, the series is said to be divergent.

Power Series and Radius of Convergence. A power series in the variable x about the point $x = a$ is an infinite sum:

$$\sum_{i=1}^{\infty} a_i (x-a)^i$$

where the a_i's are the coefficients of the power series. Earlier we showed how a series can either converge or diverge. A power series has three possibilities for convergence [1]:

Theorem: For a given power series $\sum_{i=0}^{\infty} a_i(x-a)^i$ there are only three possibilities:
i) The series converges only when $x = a$
ii) The series converges for all x
iii) There is a positive number R such that the series converges if $|x-a| < R$ and diverges if $|x-a| > R$.

The number R is called the radius of convergence of the power series. The interval of convergence of a power series is the interval that consists of all values of x for which the series converges. Note that when x is an endpoint of the interval (i.e. $|x-a| = R$) the series might converge at one or both endpoints or diverge at both endpoints.

There are many techniques which can be used to test the convergence of a series. Some of these techniques are the comparison test, ratio test, and root test. These techniques are discussed in great length in Calculus II and are not the main focus of this paper.

Taylor Series Expansions. For a generic, infinitely differentiable, function, $f(x)$, the Taylor series expansion of $f(x)$ about the point $x = a$ is:

$$T(x) = \sum_{i=0}^{\infty} \frac{f^{(i)}(a)}{i!}(x-a)^i$$

and the truncated Taylor series or Taylor polynomials are denoted:

$$T_n(x) = \sum_{i=0}^{n} \frac{f^{(i)}(a)}{i!}(x-a)^i$$

namely, the sum of the first $n+1$ terms of the Taylor series expansion.

As an example, consider the function $f(x) = e^x$ and find the Taylor series expansion about the point $x = 0$ (Figure 1). It is known that $f^{(i)}(0) = e^0 = 1,\ \forall i$ so the Taylor polynomials simplify:

$$T_n(x) = \sum_{i=0}^{n} \frac{f^{(i)}(0)}{i!}(x-0)^i = \sum_{i=0}^{n} \frac{x^i}{i!} = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \cdots \frac{x^n}{n!}$$

As another example, consider the function $f(x) = \dfrac{\cos(x)}{1+x^2}$ and find the Taylor series expansion about $a = 0$:

$$\begin{aligned} f(x) &= \sum_{i=0}^{\infty} \frac{f^{(i)}(0)}{i!}(x-0)^i \\ &= 1 - \frac{3x^2}{2} + \frac{37x^4}{24} - \frac{1111x^6}{720} + \cdots \end{aligned}$$

and again make a comparison to the original function (Figure 2).

Upon examining Figures 1 and 2, a natural question arises: Why does the Taylor polynomial approximation of $\dfrac{\cos(x)}{1+x^2}$ diverge so quickly while the Taylor polynomial approximation of e^x is so good? In order to

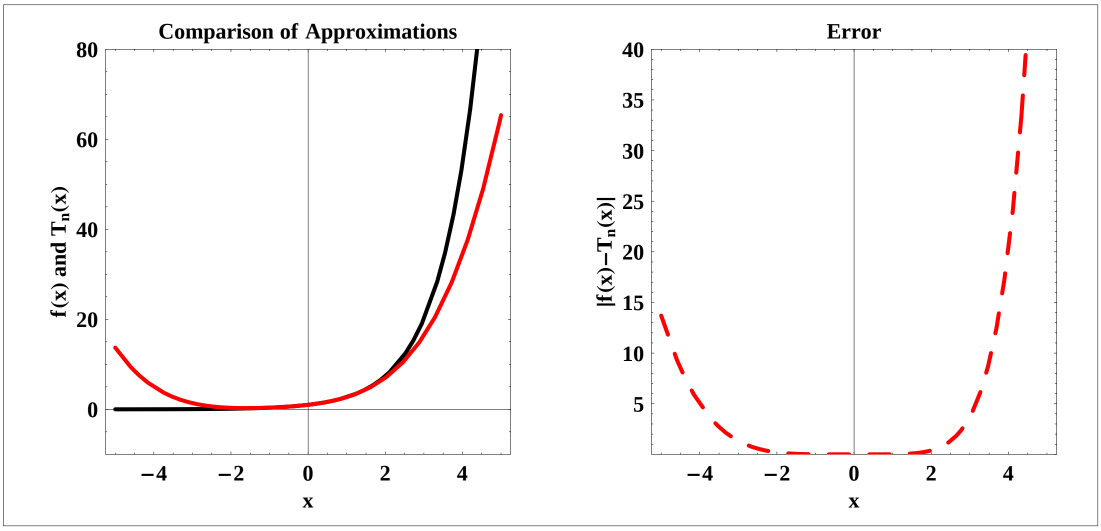

Figure 1: Comparison of $f(x) = e^x$ (black) and $T_4(x)$ (red). The functions are solid colored and the associated error is dashed.

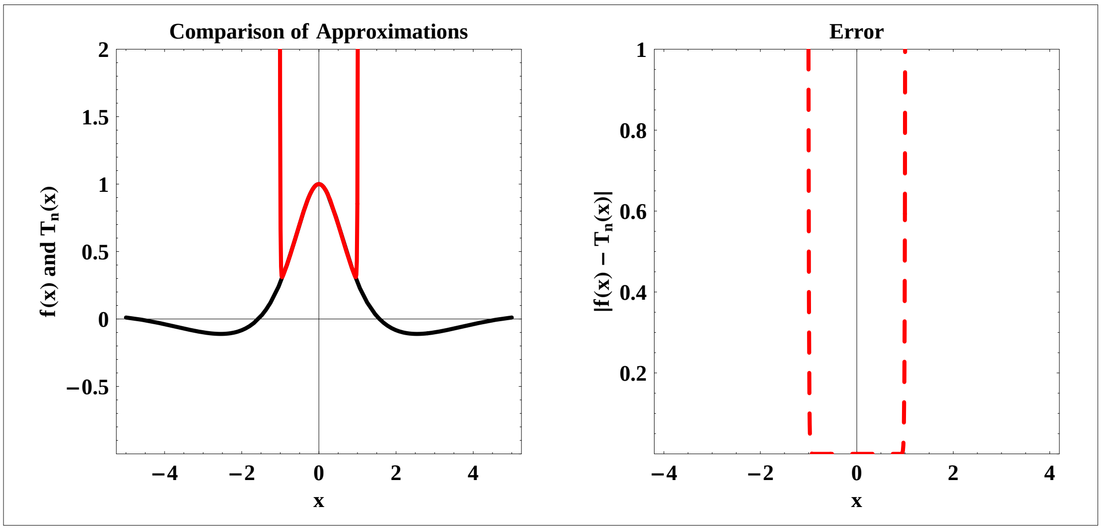

Figure 2: Comparison of $f(x) = \frac{\cos(x)}{1+x^2}$ (black) and $T_{100}(x)$ (red). The functions are solid colored and the associated error is dashed.

answer this question we must consider the radius of convergence for the two functions. To find the radius of convergence of $f(x) = e^x$ use the Ratio Test by letting $a_n = \dfrac{x^n}{n!}$:

$$\left|\frac{a_{n+1}}{a_n}\right| = \left|\frac{\left(\frac{x^{n+1}}{(n+1)!}\right)}{\left(\frac{x^n}{n!}\right)}\right| = \left|\frac{x^{n+1}n!}{(n+1)!x^n}\right| = \frac{|x|}{n+1} \longrightarrow 0 \text{ as } n \to \infty$$

Therefore, since $lim_{n\to\infty}\left|\dfrac{a_{n+1}}{a_n}\right| < 1\ \forall x \in \mathbb{R}$, the series converges $\forall x$ and the radius of convergence is $R = \infty$.

To find the radius of convergence of $f(x) = \dfrac{\cos(x)}{1+x^2}$ we can either use the method of distance to complex poles [2, 3] (where the complex poles for this function are at $\pm i$ and so the distance in the complex plane from the point of expansion to the poles is 1) or notice that $f(x)$ is can be separated as the product of two functions:

$$f(x) = \frac{\cos(x)}{1+x^2} = \cos(x)\left(\frac{1}{1+x^2}\right)$$

The Ratio Test can be used to show that the Taylor series expansion of $\cos(x)$ converges $\forall x \in \mathbb{R}$. Recognizing that $\dfrac{1}{1+x^2}$ is the geometric series we know that it has interval of convergence $\forall x \in (-1,1)$. Therefore, $\dfrac{\cos(x)}{1+x^2}$ has interval of convergence of the limiting $\forall x \in (-1,1)$.

3. PADÉ AND ALGEBRAIC APPROXIMANTS

Padé Approximants. The Taylor series expansion can be generalized to Padé approximants. Simply stated, the Padé approximant of a given power series is a rational function where the numerator is of degree L and the denominator is of degree M. If $M = 0$, the Padé approximant is equal to the Lth Taylor Polynomial (i.e. $T_L(x)$). For example, consider the power series representation of a function $f(x)$:

$$f(x) = \sum_{i=0}^{\infty} a_i x^i.$$

Then the rational function representing the Padé approximant is defined as [4]:

$$[L/M](x) = \frac{P_L(x)}{Q_M(x)} \text{ provided } Q_M(x) \neq 0$$

where

$$P_L(x) = \sum_{i=0}^{L} p_i x^i \text{ and } Q_M(x) = \sum_{i=0}^{M} q_i x^i$$

Therefore,

$$[L/M](x) = \frac{p_0 + p_1 x + p_2 x^2 + p_3 x^3 + \cdots + p_L x^L}{q_0 + q_1 x + q_2 x^2 + q_3 x^3 + \cdots + q_M x^M}$$

Examination of this equation reveals that there are $L+M+2$ unknown coefficients ($L+1$ unknown p's in the numerator and $M+1$ unknown q's in the denominator). However, defining $q_0 = 1$ leaves $L+M+1$ unknown coefficients (multiplying $[L/M](x)$ by $\dfrac{\left(\frac{1}{q_0}\right)}{\left(\frac{1}{q_0}\right)}$):

$$[L/M](x) = \frac{p_0 + p_1 x + p_2 x^2 + p_3 x^3 + \cdots + p_L x^L}{1 + q_1 x + q_2 x^2 + q_3 x^3 + \cdots + q_M x^M}$$

If the power series for $f(x)$ is known then we can write:

$$\begin{aligned} [L/M](x) = \frac{P_L(x)}{Q_M(x)} &\cong f(x) \\ Q_M(x) f(x) - P_L(x) &\cong 0 \\ Q_M(x)\left(\sum_{i=0}^{L+M+1} a_i x^i\right) - P_L(x) &\cong 0 \end{aligned} \tag{1}$$

It is now possible to solve the system of $L+M+1$ equations for the $L+M+1$ unknown coefficients by equating coefficients of powers of x to zero and solving the resulting system of equations. There are $L+M+1$ because we need to have the expansion of the function to at least that many terms in order to capture all of the contributions of smaller powers of x in the coefficients. Once the p's and q's in $P_L(x)$ and $Q_M(x)$ are determined we can solve Eq.(1) for $f(x)$:

$$f(x) = \sum_{i=0}^{\infty} a_i x^i \cong \frac{P_L(x)}{Q_M(x)} = [L/M](x)$$

In this way, when the power series of $f(x)$ is known, the function $f(x)$ can be approximated by a Padé approximant. Generating Padé approximants in this manner is not only computationally time consuming but it is also inconvenient because each new Padé approximant requires the solving of a new system of $L+M+1$ equations for the $L+M+1$ unknowns. This is not a large problem with the computers of today but it still takes considerable time to compute the Padé approximant for large L and M. There are ways to compute $[L/M](x)$ for various L and M using continued fractions, however, these methods are not the focus of this paper.

It is common practice to display the approximants in a table, called a Padé table (Table 1). It is important to note that it is the diagonal terms of the Padé table that are used to see the convergence of the Padé approximants. Convergence occurs as L and $M \to \infty$ (i.e. $f(x) = \lim_{M\to\infty, L\to\infty} [L/M](x)$). The convergence of the Padé approximant will be discussed later in conjunction with the convergence of the Algebraic approximant. Notice that for the first column of the Padé table (where $M = 0$ and $L = n$); the Padé approximant is equal to the Taylor polynomial, $T_n(x)$ (the second column is the first column of the Aitken's Delta-Squared Process [5]):

$$[L/0](x) = \frac{P_L(x)}{Q_0(x)} = p_0 + p_1 x + p_2 x^2 + p_3 x^3 + \cdots + p_L x^L = T_L(x).$$

		M					
		0	1	2	3	$\cdots$	M
L	0	[0/0]	[0/1]	[0/2]	[0/3]	$\cdots$	[0/M]
	1	[1/0]	[1/1]	[1/2]	[1/3]	$\cdots$	[1/M]
	2	[2/0]	[2/1]	[2/2]	[2/3]	$\cdots$	[2/M]
	3	[3/0]	[3/1]	[3/2]	[3/3]	$\cdots$	[3/M]
	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
	L	[L/0]	[L/1]	[L/2]	[L/3]	$\cdots$	[L/M]

Table 1: Generic Padé Table.

Comparison with Taylor Series Expansion. Recall that earlier we compared the Taylor series expansions of $f(x) = e^x$ and $f(x) = \dfrac{\cos(x)}{1+x^2}$ to the functions. Now, a comparison of these functions with the Padé approximants can be seen in Figure 3 where $n = 4$ for the Taylor series expansion of $f(x) = e^x$, $n = 100$ for the Taylor series expansion of $f(x) = \dfrac{\cos(x)}{1+x^2}$ and n is only 4 for both of the Padé approximants. Notice that the Padé approximant approximates the function even outside the interval ov convergence of the Taylor series, where the Taylor series expansion diverges from the function. Also, only 4 terms were used in the Padé approximant whereas 100 terms were used in the Taylor series expansion. Meaning that 100 derivatives of $f(x)$ were calculated in order to get $T_{100}(x)$ and to calculate $[4/4](x)$ only required solving a system of 9 equations for the 9 unknown p's and q's.

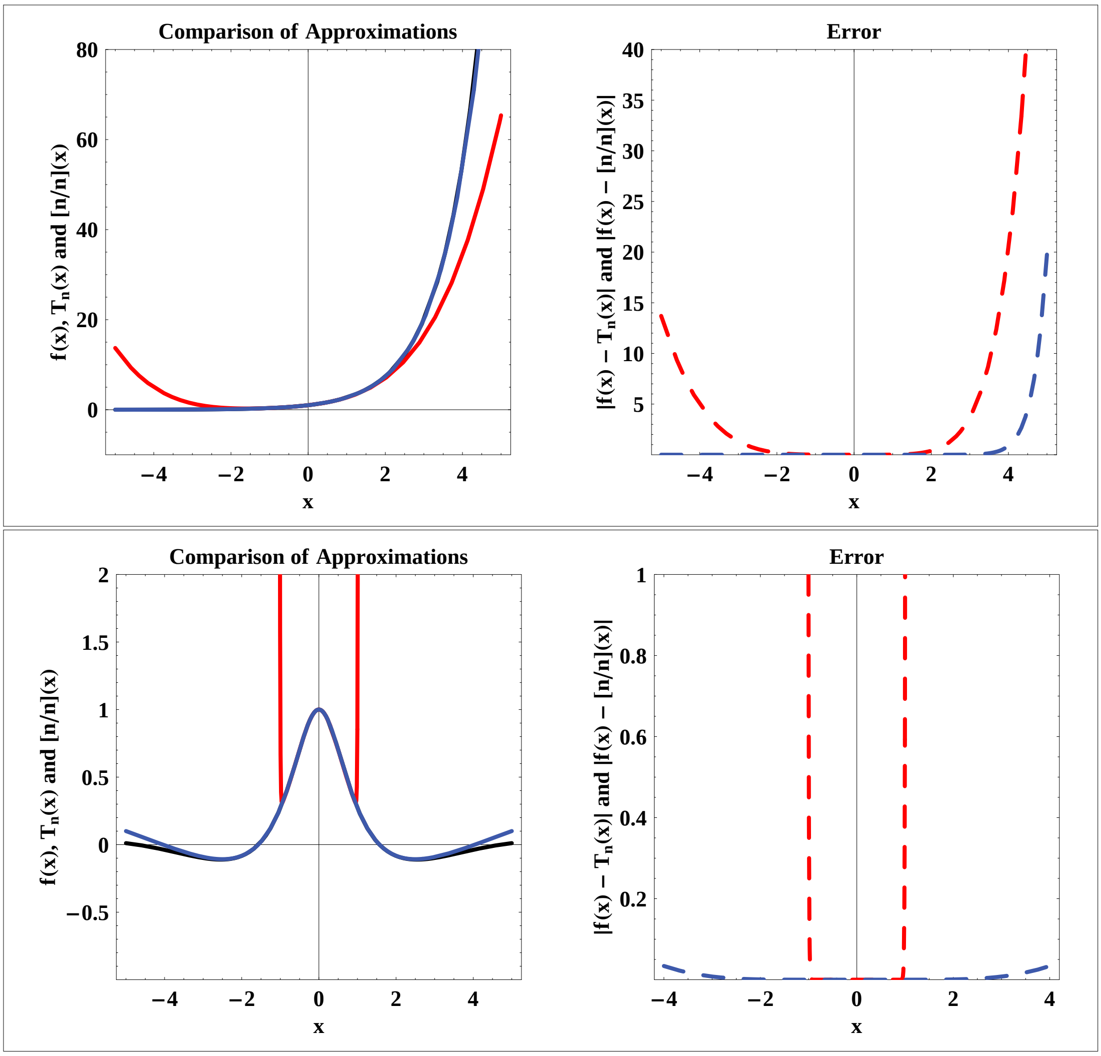

Figure 3: Top: Comparison of $f(x) = e^x$ (black), $T_4(x)$ (red), and $[4,4](x)$ (blue). Bottom: Comparison of $f(x) = \frac{\cos(x)}{1+x^2}$ (black), $T_{100}(x)$ (red), and $[4,4](x)$ (blue). Again, the functions are solid colored and their associated errors are dashed.

Another power of Padé approximants is that the Taylor series approximates polynomials with finite series whereas Padé approximants approximate rational functions by rational finite series. An example of this is that $\frac{1}{1+x^2}$ is an infinite series in the Taylor Polynomials, but is exactly determined by the Padé approximant.

Extension to Algebraic Approximants. Consider the definition of a Padé approximant as we had it defined before:

$$[L/M](x) = \frac{P_L(x)}{Q_M(x)}$$

which lead to the Eq. (1). Notice that in Eq. (1) $[L/M](x)$ is real-valued and thus will only be able to assign real values to an infinite series. If we are expecting to have complex-valued sums we will need to use a different approximation to find them. The extension of the Padé approximant to the Algebraic approximants [4, 6] done by adding a squared term to Eq. (1). The Algebraic approximant of a given power series ($f(x) = \sum_{i=0}^{\infty} a_i x^i$) is denoted by $[L/M/N](x)$ and is a function of three polynomials ($P_L(x), Q_M(x), R_N(x)$):

$$P_L(x) - Q_M(x)\left(\sum_{i=0}^{\infty} c_i x^i\right) + R_N(x)\left(\sum_{i=0}^{\infty} c_i x^i\right)^2 = 0 \tag{2}$$

where

$$P_L(x) = \sum_{i=0}^{L} p_i x^i,\ Q_M(x) = \sum_{i=0}^{M} q_i x^i \text{ and } R_N(x) = \sum_{i=0}^{N} r_i x^i$$

Again, setting coefficients of powers of x equal to 0 in Eq. (2) and solving the resulting system of equations for the coefficients in the polynomials $P_L(x)$, $Q_M(x)$, and $R_N(x)$ it becomes possible to assign a "sum" to the power series $f(x) = \sum_{i=0}^{\infty} a_i x^i$. Solving Eq. (2) for $f(x)$:

$$\begin{aligned} f(x) = \left(\sum_{i=0}^{\infty} a_i x^i\right) \cong [L/M/N](x) &= \frac{Q_M(x) \pm \sqrt{Q_M(x)^2 - 4R_N(x)P_L(x)}}{2R_N(x)} \\ &= \frac{Q_M(x)}{2R_N(x)} \pm \sqrt{\frac{Q_M(x)^2 - 4R_N(x)P_L(x)}{4R_N(x)^2}} \\ &= \frac{Q_M(x)}{2R_N(x)} \pm \sqrt{\frac{Q_M(x)^2}{4R_N(x)^2} - \frac{P_L(x)}{R_N(x)}} \end{aligned}$$

Convergence. As stated earlier, that convergence of the Padé approximant occurs as L and $M \to \infty$ (i.e. $f(x) = \lim_{M\to\infty, L\to\infty} [L/M](x)$). It can also be shown that the Algebraic approximant converges to the function as $L, M, N \to \infty$. There are no rigorous convergence results for these ideas. However, there are multiple theorems [4] that do address the issue for specific functions. One example is:

> Theorem: Let $f(z)$ be analytic at the origin, and also in the circle $|z| \le R$, except for m poles, counting multiplicity. Consider a sequence $[L_k, M_k]$ of Padé Approximants of $f(z)$ with $M_k \ge m$ and $L_k/M_k \to \infty$ as $k \to \infty$ ($M_k \ne 0$). Let ε, δ be arbitrarily small positive given numbers. Then k_0 exists such that $|f(z) - [L_k, M_k]| < \varepsilon$ for all $k > k_0$ and all $|z| \le R$ except for $z \ni \xi$, where ξ is a set of points of the z-plane of measure less than δ.

The problem with using theorems like this one to prove the convergence of the Padé approximant is that it assumes that we know something about the function, ($f(x)$); this is not always the case.

The true beauty of the Padé and Algebraic approximants is not fully understood until you consider that this formalism can be used to determine the value of an unknown function, $f(x)$, provided it's power series, $\sum a_i x^i$, is known. An example of where this occurs can be found in the quantum anharmonic oscillator.

4. QUANTUM MECHANICS

Quantum Mechanics. As stated earlier, one of the key ideas in quantum mechanics is to solve the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2}+\frac{1}{2}m\omega^2x^2\Psi(x)=E\Psi(x)$$

for the wavefunction, $\Psi(x)$, and the energy, E. In the remainder of this paper I will focus on solving the Schrödinger equation for the energy.

Schrödinger Equation. Simply stated, the Schrödinger equation plays the role of Newton's laws and conservation of energy in classical mechanics by predicting the future behavior of a dynamical, quantum system. Imagine a particle of mass m confined to move along the x-axis and under the influence of a force, $F(x,t)$. In classical mechanics Newton's second law ($F=ma$) and the appropriate initial conditions ($x(0)$ and an initial velocity) are used to determine the position of the particle, $x(t)$ and then all the other dynamical variables (velocity, momentum, kinetic energy, etc.) are calculated. In quantum mechanics, however, the desired quantity is the wave equation, $\Psi(x,t)$, of the particle. It is this wave equation which predicts analytically and precisely the probability of events or outcomes. The detailed outcome is not strictly determined, but given a large number of events, the Schrödinger equation will predict the distribution of events. In the Schrödinger equation, the kinetic and potential energies are transformed into the Hamiltonian which acts on the wavefunction to generate the evolution of the system in time and space. The Schrödinger equation gives the quantized energies of the sytem so that other properties may be calculated.

The Schrödinger equation can also be written in bra/ket notation:

$$\hat{H}|\Psi\rangle=E|\Psi\rangle$$

where $\hat{H}$ is the Hamiltonian:

$$\left(\frac{1}{2}\hat{p}^2+V(x)\right)|\Psi\rangle=E|\Psi\rangle$$

where $p^2=-\frac{d^2}{dx^2}$, $V(x)$ is the potential, and E is the energy eigenvalue for the system.

The Schrödinger Equation is simply a second order variable coefficient ordinary differential equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2}+\frac{1}{2}m\omega^2x^2\Psi(x)=E\Psi(x)$$

Harmonic Oscillator. Consider the simple harmonic oscillator. The typical, classical harmonic oscillator consists of a mass, m, attached to a spring with spring constant k. The motion of this system, ignoring friction and other effects (as usual), is governed by Hooke's Law:

$$F = -kx = m\frac{d^2x}{dt^2}$$

which is a second order differential equation with solution

$$x(t) = A\sin(\omega t) + B\cos(\omega t)$$

where ω is defined as $\sqrt{\frac{k}{m}}$ and is nothing more than the angular frequency of oscillation. Furthermore, we know that the potential, $V(x)$, is:

$$V(x) = -\int F\,dx = \frac{1}{2}kx^2$$

Notice that $V(x)$ is nothing more than a parabola.

The quantum mechanical harmonic oscillator is slightly different. We still consider a system consisting of a mass, m, attached to a spring with spring constant k. However, here we solve the Schrödinger equation for the potential:

$$V(x) = \frac{1}{2}m\omega^2x^2.$$

Substituting into the time independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + \frac{1}{2}m\omega^2x^2\Psi(x) = E\Psi(x)$$

There are two basic ways to solve this equation, algebraic and analytic (see [7] pages 32-44 for derivation). Regardless of the method, the solution is:

$$\Psi_n(x) = \left(\frac{m\,\omega}{\pi\,\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n(\zeta) e^{\frac{-\zeta^2}{2}}$$

where the $H_n(\zeta)$ are the Hermite polynomials.

However, it is obvious that there is no such thing as a frictionless harmonic oscillator. This is why perturbation theory is so important. Perturbation theory can be thought of as a composition of a general mathematical method developed to deal with small fluctuations or corrections in a system and is often used to approximate a solution to a problem which cannot be solved exactly starting from the solution to the unperturbed problem [8]. Perturbation theory results in series expansions for quantities. In many cases, the resulting series is divergent.

5. FINDING RECURRENCE RELATIONS FOR THE POTENTIAL USED IN ARDA [9]

Hypervirial and Hellmann-Feynman Theorems. (Descriptions and Proofs in Appendix A). One example of where perturbation theory is used is in using the Hypervirial and Hellmann-Feynman Theorems [8] to determine the energy eigenvalue, E, for the Schrödinger equation. The Hypervirial theorem states that the expectation value of any Hamiltonian and any other operator is zero and the Hellmann-Feynman Theorem shows how to relate changes in the parameters of the Hamiltonian to changes that can be expected in the energy. Using the Hamiltonian presented by Arda [9] to describe the anharmonic oscillator with potential $V(x) = \frac{1}{2}\omega^2 x^2 + \frac{1}{2}\lambda x^2 + \lambda^2 x^3$ (Figure 4). Then the Schrödinger equation ($\hat{H}|\Psi\rangle = E|\Psi\rangle$):

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}\omega^2 x^2 + \frac{1}{2}\lambda x^2 + \lambda^2 x^3\right)|\Psi\rangle = E|\Psi\rangle$$

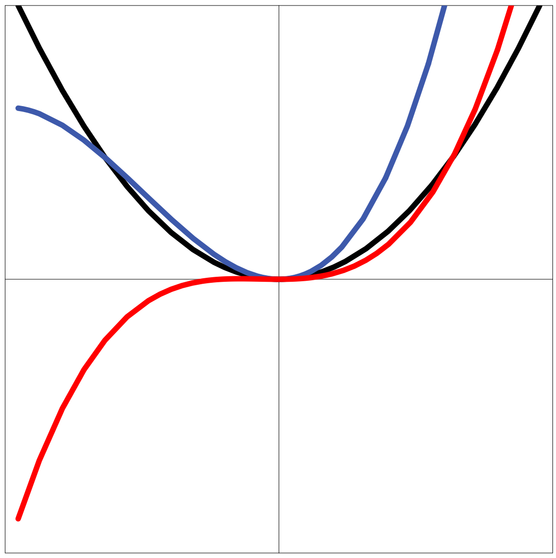

Figure 4: Graphical representation of the potential presented in Arda [9] for perturbation $\lambda = 0.75$ (cobalt), $\lambda = -0.75$ (red), and the harmonic oscillator where $\lambda = 0$ (black).

Setup and Derivation. There are many key ideas that need to be carefully implemented in order to find the complete recurrence relations describing the coefficients in the expansion of the energy. Some of these ideas include expanding the Hypervirial Theorem by using the Schrödinger equation and multiple commutator relations from quantum mechanics and using Hellmann-Feynman Theorem for further simplifications. Once an equation for the energy is reached, assume a power series solution for the energy:

$$E = \sum_{k=0}^{\infty} E_n^{(k)} \lambda^k$$

where for $k = 0$, $E = E_n^{(0)} = \hbar\omega\left(n + \frac{1}{2}\right)$ and expanding the expectation value for x^s:

$$\int_0^{\infty} \Psi*(x) x^s \Psi(x) dx = \sum_{k=0}^{\infty} A_s^{(k)} \lambda^k$$

when $s = 1$, $1 = \sum_{k=0}^{\infty} A_s^{(k)} \lambda^k$. If $A_0^{(0)} = 1$ then $A_0^{(k)} = 0\ \forall k \neq 0$. Set coefficients of like powers of λ equal to 0 (this process is an extension of series solutions [2]). Doing the complete derivation is a long process (see Appendix B for details), however, it is possible to find that the recurrence relations are:

$$
\begin{aligned}
A_s^{(0)} &= \frac{2(s-1)}{s}\frac{1}{\omega^2}\left[\frac{1}{8}(s-2)(s-3)A_{s-4}^{(0)}+E_n^{(0)}A_{s-2}^{(0)}\right]\\
A_s^{(1)} &= \frac{2(s-1)}{s}\frac{1}{\omega^2}\left[-\frac{s}{2(s-1)}A_s^{(0)}+\frac{1}{8}(s-2)(s-3)A_{s-4}^{(1)}+E_n^{(0)}A_{s-2}^{(1)}+E_n^{(1)}A_{s-2}^{(0)}\right]\\
A_s^{(r)} &= \frac{2(s-1)}{s}\frac{1}{\omega^2}\\
&\quad \left[-\frac{2s+1}{2(s-1)}A_{s+1}^{(r-2)}-\frac{s}{2(s-1)}A_s^{(r-1)}+\frac{1}{8}(s-2)(s-3)A_{s-4}^{(r)}+\sum_{i=0}^{r}E_n^{(i)}A_{s-2}^{(r-i)}\right] \text{ for } r=2,3,4,\ldots\\
E_n^{(0)} &= \hbar\omega\left(n+\frac{1}{2}\right)\\
E_n^{(1)} &= \frac{1}{2}A_2^{(0)}\\
E_n^{(r)} &= \frac{1}{2(r)}A_2^{(r-1)}+\frac{2}{(r)}A_3^{(r-2)} \text{ for } r=2,3,4,\ldots
\end{aligned}
$$

These recurrence relations are used to generate the coefficients in the expansions of the energy, $E=\sum_{i=0}^{n}E_n^{(i)}\lambda^i$. The result is an infinite power series in the perturbation parameter λ. In the end, what we want are the values of the $E_n^{(i)}$. Yet, all the other equations are necessary to determine these values. In this case, the resulting series is divergent for most values of λ. The first few terms in the expansion of the energy are:

$$
E(\lambda)=\frac{1}{2}+\frac{\lambda}{4}-\frac{\lambda^2}{16}+\frac{\lambda^3}{32}-\frac{357\lambda^4}{256}+\frac{1415\lambda^5}{512}-\frac{8469\lambda^6}{2048}+\frac{22561\lambda^7}{4096}-\frac{1403309\lambda^8}{65536}+\frac{9652939\lambda^9}{131072}-\frac{99328383\lambda^{10}}{524288}
$$

$$
+\frac{420083815\lambda^{11}}{1048576}-\frac{88343866641\lambda^{12}}{8388608}+\frac{57499714339\lambda^{13}}{16777216}-\frac{715905994109\lambda^{14}}{67108864}+\frac{3895679271393\lambda^{15}}{134217728}+\cdots \quad (3)
$$

and can be depicted graphically (Figure 5) to see that the function is indeed divergent for most values of λ. Also, the coefficients themselves are divergent (Figure 6).

6. NUMERICAL RESULTS

Mathematica. Once the recurrence relations are found they can be implemented in *Mathematica* to numerically calculate the coefficients in the expansion of the energy. The coefficients can then be used to initialize the Padé and Algebraic approximants and a meaningful "sum" can be assigned to the series. This process is very similar to what we did earlier for the Taylor series expansion where we initialized the Padé and Algebraic approximants with the terms of the Taylor series which came from successive derivatives of the known function. However, in the case of the recurrence relations we don't know the function, the series expansion of the energy is divergent, and we are still able to assign a value to the function!

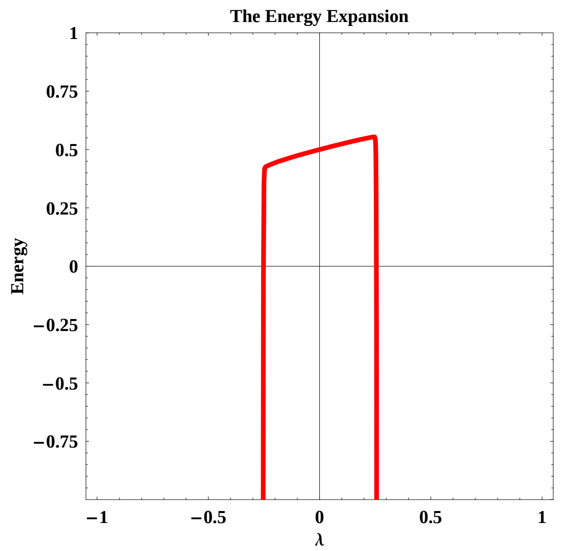

Figure 5: The first 200 terms in the power series expansion of the energy.

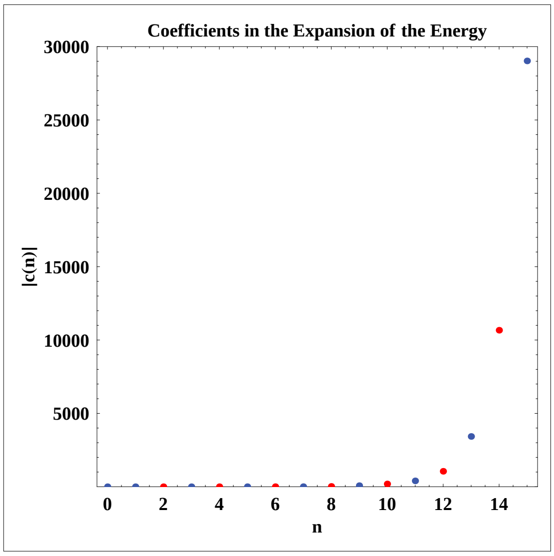

Figure 6: Absolute value of the first fifteen coefficients in the expansion of the energy, $E = \sum_{i=0}^{n} E_n^{(i)} \lambda^i$. The positive coefficients are shown as blue points and the negative coefficients are shown as red points.

Data. For example, consider the case where $\lambda = 0.3$. Then we can use the Padé approximant to construct a Padé Table (Table 2). Recalling that we expect to see convergence along the diagonal we can see that the energy for this particular perturbation of λ is approaching 0.5631744.

L \ M	0	1	2	3	4	5	6
0	0.50000000	0.57010869	0.56349749	0.56319165	0.56317553	0.56317444	0.56317441
1	0.57500000	0.56943364	0.56357162	0.56318442	0.56317489	0.56317440	0.56317441
2	0.56937500	0.56313475	0.56313386	0.56317885	0.56317487	0.56317428	0.56317441
3	0.57021875	0.56355813	0.56316652	0.56317755	0.56317462	0.56317441	0.56317441
4	0.57021875	0.56348485	0.56320869	0.56317544	0.56317456	0.56317442	0.56317441
5	0.56563876	0.56318024	0.56300908	0.56317581	0.56317450	0.56317442	0.56317441
6	0.56262416	0.56313733	0.56316903	0.56317487	0.56317446	0.56317441	0.56317441

Table 2: Part of the Padé Table for $\lambda = 0.3$ in the divergent series given above (Eq. (3)).

Now consider another value of λ, say $\lambda = -0.3$, and use the Algebraic approximant instead of the Padé approximant. Notice now that if we allow λ to be a negative number we fundamentally change the series expansion of the energy (Eq. (3)). With negative values of λ the power series expansion of the energy becomes

$$E(\lambda) = \frac{1}{2} - \frac{\lambda}{4} - \frac{\lambda^2}{16} - \frac{\lambda^3}{32} - \frac{357\lambda^4}{256} - \frac{1415\lambda^5}{512} - \frac{8469\lambda^6}{2048} - \frac{22561\lambda^7}{4096} - \frac{1403309\lambda^8}{65536} - \frac{9652939\lambda^9}{131072} - \cdots.$$

It would be useful to examine the first terms in the Padé Table as we did for $\lambda = 0.3$, but in order to construct such a table for the Algebraic approximant we would need a three dimensional array of values, a separate dimension for each of L, M, and N. Therefore, since we expect convergence to occur on the diagonal; consider the case where $L = M = N$ (Table 3). Notice that after a certain value of L, M, N is reached we get a complex value for the energy, $E(\lambda)$.

Now if we consider all values of $\lambda \in (-1, 1)$ (λ is taken from -1 to 1 because in quantum mechanics the perturbation is often thought of as being either on or off) we can see how different values of λ give different solutions of the energy. First, using the coefficients in the expansion of the energy, Eq. (3), to initialize the Padé approximant. Comparing the Padé and Algebraic approximants to the first 200 terms in the expansion of the energy (Figure 7) shows that all three approximations are converging to the value of the energy for small values of λ. Furthermore, it becomes evident that the Algebraic approximant found the complex part of the energy where the Padé approximant fails. There are values of λ where we will get real solutions and other regions where complex solutions exist. The complex part of the energy is related to the lifetime of the state. This can be explained by realizing that the because the Padé approximant is defined by a linear equation, Eq. (1), there is no possibility to find a complex valued sum. Whereas the Algebraic approximant is a quadratic function, Eq. (2), and thus allows for the possibility of complex results. A comparison of various Algebraic approximants for the energy are shown in Figure 8. The true value of the energy exists at the overlap of the approximants because convergence occurs as $L, M, N \to \infty$ successive overlays of approximants will approximate the energy better than the last.

7. CONCLUSIONS

The Padé and Algebraic approximants were used to both approximate known functions ($\frac{\cos(x)}{1+x^2}$ and e^x) by initializing the approximants with the coefficients of the Taylor series expansion. Furthermore, the Padé and

L,M,N	$[L/M/N]$	
0	0.5000000000	0.5000000000
1	0.4971671153	0.4189382124
2	0.4260293212	0.4126563658
3	0.5996869791	0.3886596504
4	0.3858466474	0.3438295662
5	0.3857874106	0.3453904712
6	0.3822819828	0.3741246435
7	0.3869280073 + 0.0062323054 i	0.3869280073 - 0.0062323054 i
8	0.3868241723	0.3818008106
9	0.3851494634 + 0.0028742112 i	0.3851494634 - 0.0028742112 i
10	0.3856097646 + 0.0034022507 i	0.3856097646 - 0.0034022507 i
11	0.3859178893 + 0.0024980798 i	0.3859178893 - 0.0024980798 i
12	0.3864275478 + 0.0031498306 i	0.3864275478 - 0.0031498306 i
13	0.3864844461 + 0.0029409675 i	0.3864844461 - 0.0029409675 i
14	0.3864660602 + 0.0029275643 i	0.3864660602 - 0.0029275643 i
15	0.3865782297 + 0.0028786517 i	0.3865782297 - 0.0028786517 i
20	0.3865105657 + 0.0028138232 i	0.3865105657 - 0.0028138232 i
40	0.3864700370 + 0.0027872350 i	0.3864700370 - 0.0027872350 i
60	0.3864700482 + 0.0027872827 i	0.3864700482 - 0.0027872827 i

Table 3: Part of the diagonal of the "Padé Table" for $\lambda = -0.3$ in the expansion of the energy, Eq. (3).

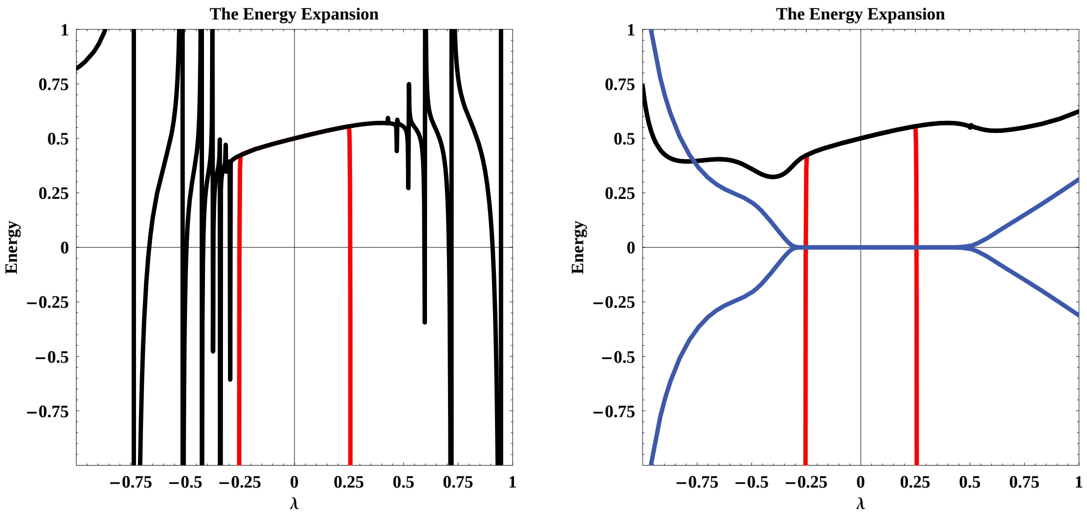

Figure 7: Left: Comparison of the first 200 terms in the expansion of the energy, $E(\lambda)$, (red) and $[20/20](\lambda)$ (black). Right: Comparison of the first 200 terms in the expansion of the energy, $E(\lambda)$, (red) and $[20/20/20](\lambda)$. The real part of $[20/20/20](\lambda)$ is black and the complex part is blue.

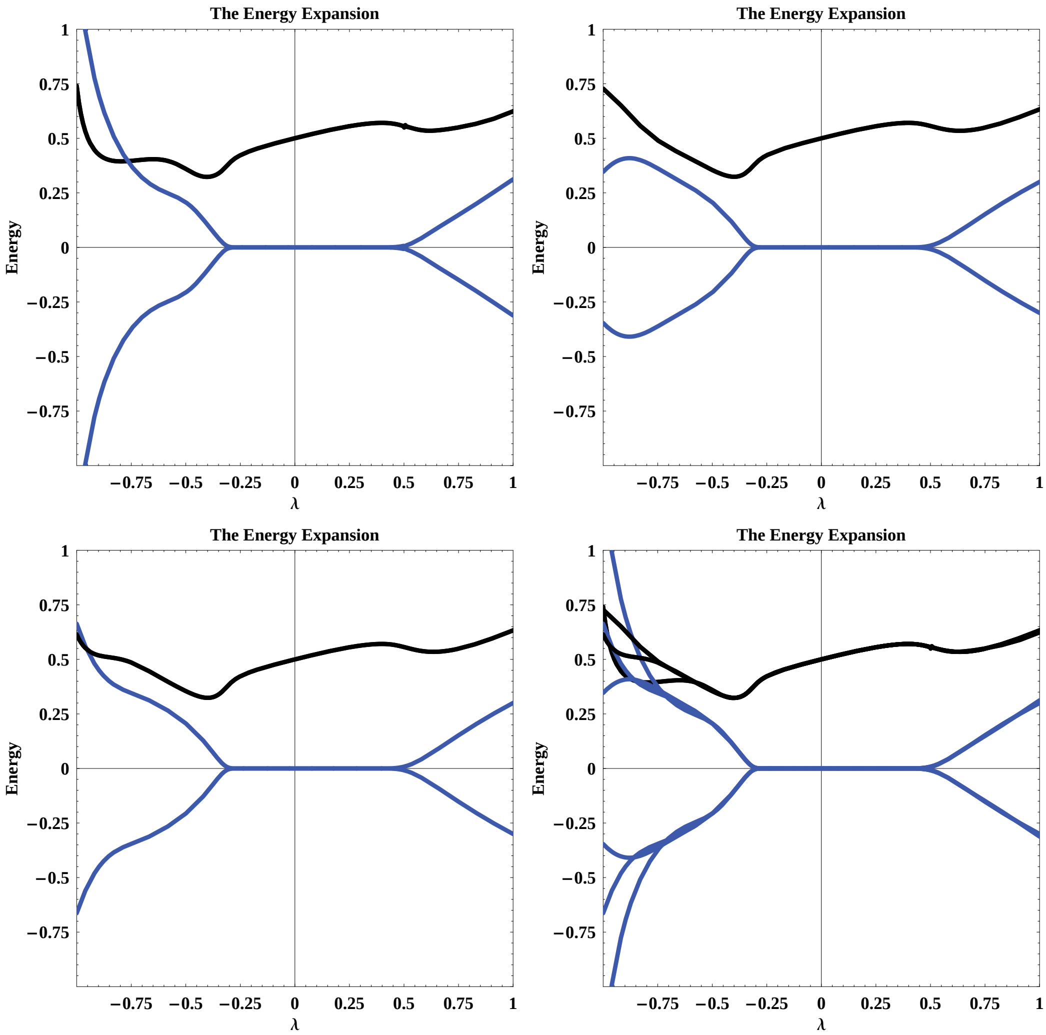

Figure 8: Comparison of Algebraic approximants. Top: [20/20/20](λ) (left) and [40/40/40](λ) (right). Bottom: [60/60/60](λ) (left) and an overlay of [20/20/20](λ), [40/40/40](λ), and [60/60/60](λ) (right). The black lines are the real part of the energy and the blue lines are the imaginary parts. The true value of the energy occurs at the overlap of the functions.

Algebraic approximants were used to approximate the unknown energy for the quantum anharmonic oscillator through initialization from the coefficients in the expansion of the energy. Both the Padé and Algebraic approximants have been used to determine a function when only the divergent power series for the function was known!

There are also many examples where both the Padé and Algebraic approximants do "strange" things. For example, applying Padé approximants to the Fibonacci Sequence $(1+1+2+3+5+8+13+21+34+55+\ldots)$ yields a sum of -1.0! A surprising solution since this is a sum of positive integers. Also, using the Algebraic approximant on the series expansion of $\ln(x)$ gives a complex value for $x=-1$ (i.e. $\ln(-1)=i\pi$).

Future Work. One issue with this method of using Padé and Algebraic approximants to assign sums to divergent series is that there are few other ways of checking the convergence of the solutions. To check the sums it is necessary to check them against sums for the same problem using a different method. There are other methods of assigning a sum to a divergent series including the Borel Method of Resummation [10] and Aitken's Delta-Squared Method. However, to date, no one has used the Borel Method of Resummation when dealing with the quantum anharmonic oscillator so there is no existing data to compare results and Aitken's Delta-Squared Method fails to give the complex results. The next step would be to implement the Borel Method of Resummation and check to see that all three methods (Padé approximants, Algebraic approximants, and the Borel Method of Resummation) give the same result.

Appendix A:

THE HYPERVIRIAL AND HELLMANN-FEYNMAN THEOREMS

THE HYPERVIRIAL THEOREM. Simply stated, the Hypervirial Theorem says that the expectation value of any Hamiltonian, $\hat{H}$, and any other time-independent operator, $\hat{O}$, is zero.

$$\left\langle \Psi \middle| [\hat{H},\hat{O}] \middle| \Psi \right\rangle = 0$$

Proof. Consider a system in the stationary state Ψ and let $\hat{H}$ be its time-independent Hamiltonian. Then if $\hat{O}$ is any time-independent linear operator, by the definition of commutators:

$$\left\langle \Psi \middle| [\hat{H},\hat{O}] \middle| \Psi \right\rangle = \left\langle \Psi \middle| \left(\hat{H}\hat{O} - \hat{O}\hat{H}\right) \middle| \Psi \right\rangle = \left\langle \Psi \middle| \hat{H}\hat{O} \middle| \Psi \right\rangle - \left\langle \Psi \middle| \hat{O}\hat{H} \middle| \Psi \right\rangle$$

Proving this for a general Hamiltonian is difficult and involves Green's Theorem and other ideas. However, the Hamiltonian used in this paper is Hermitian. Thus:

$$\left\langle \Psi \middle| \hat{H}\hat{O} \middle| \Psi \right\rangle = \left\langle \Psi \middle| \hat{O}\hat{H} \middle| \Psi \right\rangle$$

and therefore we immediately have the Hypervirial Theorem:

$$\left\langle \Psi \middle| [\hat{H},\hat{O}] \middle| \Psi \right\rangle = 0$$

THE HELLMANN-FEYNMAN THEOREM. "[T]here are some who feel that the identity is too trivial to merit the term "theorem," the present appelation does preserve for us the name of Hellmann who early in his career lost his life in the Stalinist purges" (see [11] for more information). Unknown to each other, Hellmann derived this equation in a textbook and Feynman in an article [11] which was based on part his undergraduate thesis at MIT entitled: "Stresses in Molecules". Both were writing about forces in molecules, which, in quantum mechanics, are unobservable.

Nevertheless, the Hellmann-Feynman Theorem shows how to relate changes in the parameters of the Hamiltonian to changes that can be expected in the energy:

$$\frac{\partial E}{\partial \lambda} = \left\langle \Psi \middle| \frac{\partial \hat{H}}{\partial \lambda} \middle| \Psi \right\rangle$$

where λ is a parameter in the Hamiltonian (e.g. $\hat{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}\omega^2 x^2 + \frac{1}{2}\lambda x^2 + \lambda^2 x^3$) and $< \Psi|...|\Psi >$ denotes the quantum-mechanical expectation value. Some examples of the quantum-mechanical expectation value are:

$$\langle \Psi | x | \Psi \rangle = \langle x \rangle = \int \Psi^*(x)\Psi dx$$

$$\langle \Psi | p | \Psi \rangle = \langle p \rangle = \int \Psi^* \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) \Psi dx = -i\hbar \int \Psi^* \left(\frac{\partial \Psi}{\partial x}\right) dx$$

Proof. To prove this theorem we must first consider a system with a time-independent Hamiltonian, $\hat{H}$, that involves parameters. The Hamiltonian of any system contains parameters and therefore we can consider the one-dimensional harmonic oscillator Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2$$

Here, the force constant, k, and the mass, m, are both parameters. And, the stationary-state energies, E_n, are functions of the same parameters:

$$E_n = (n+\frac{1}{2})\hbar\omega = (n+\frac{1}{2})\hbar\left(\frac{k}{m}\right)^{\frac{1}{2}}.$$

Again, the Hellmann-Feynman Theorem shows how to relate changes in the parameters of the Hamiltonian to changes that can be expected in the energy. Let λ be one of the parameters in the Hamiltonian (i.e. $\hat{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}\omega^2 x^2 + \frac{1}{2}\lambda x^2 + \lambda^2 x^3$) and investigate the quantity $\frac{\partial E}{\partial \lambda}$. Starting with the Schrödinger equation:

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

where $\hat{H}$ are the eigenvectors and E is the associated eigenvalue of the transformation. Then multiplying both sides of the Schrödinger equation by $\langle\Psi|$ and taking the derivative with respect to λ:

$$\frac{\partial}{\partial\lambda}\langle\Psi|\hat{H}|\Psi\rangle = \frac{\partial}{\partial\lambda}\langle\Psi|E|\Psi\rangle.$$

Invoking the Chain Rule:

$$\left\langle\frac{\partial\Psi}{\partial\lambda}\middle|\hat{H}\middle|\Psi\right\rangle + \left\langle\Psi\middle|\frac{\partial\hat{H}}{\partial\lambda}\middle|\Psi\right\rangle + \left\langle\Psi\middle|\hat{H}\middle|\frac{\partial\Psi}{\partial\lambda}\right\rangle = \left\langle\frac{\partial\Psi}{\partial\lambda}\middle|E\middle|\Psi\right\rangle + \left\langle\Psi\middle|\frac{\partial E}{\partial\lambda}\middle|\Psi\right\rangle + \left\langle\Psi\middle|E\middle|\frac{\partial\Psi}{\partial\lambda}\right\rangle$$

and realizing that E does not effect $\langle\Psi|$ nor $|\Psi\rangle$ and can be taken out:

$$\left\langle\frac{\partial\Psi}{\partial\lambda}\middle|\hat{H}\middle|\Psi\right\rangle + \left\langle\Psi\middle|\frac{\partial\hat{H}}{\partial\lambda}\middle|\Psi\right\rangle + \left\langle\Psi\middle|\hat{H}\middle|\frac{\partial\Psi}{\partial\lambda}\right\rangle = E\left\langle\frac{\partial\Psi}{\partial\lambda}\middle|\Psi\right\rangle + \frac{\partial E}{\partial\lambda}\langle\Psi|\Psi\rangle + E\left\langle\Psi\middle|\frac{\partial\Psi}{\partial\lambda}\right\rangle.$$

Now, due to normalization ($\langle\Psi|\Psi\rangle = \int_{-\infty}^{\infty}|\Psi(x,t)|^2 dx = 1$), we can solve the equation for $\frac{\partial E}{\partial\lambda}$:

$$\left\langle\frac{\partial\Psi}{\partial\lambda}\middle|\hat{H}\middle|\Psi\right\rangle + \left\langle\Psi\middle|\frac{\partial\hat{H}}{\partial\lambda}\middle|\Psi\right\rangle + \left\langle\Psi\middle|\hat{H}\middle|\frac{\partial\Psi}{\partial\lambda}\right\rangle = E\left\langle\frac{\partial\Psi}{\partial\lambda}\middle|\Psi\right\rangle + \frac{\partial E}{\partial\lambda} + E\left\langle\Psi\middle|\frac{\partial\Psi}{\partial\lambda}\right\rangle.$$

$$\frac{\partial E}{\partial\lambda} = \left\langle\frac{\partial\Psi}{\partial\lambda}\middle|\hat{H}\middle|\Psi\right\rangle + \left\langle\Psi\middle|\frac{\partial\hat{H}}{\partial\lambda}\middle|\Psi\right\rangle + \left\langle\Psi\middle|\hat{H}\middle|\frac{\partial\Psi}{\partial\lambda}\right\rangle - E\left\langle\frac{\partial\Psi}{\partial\lambda}\middle|\Psi\right\rangle - E\left\langle\Psi\middle|\frac{\partial\Psi}{\partial\lambda}\right\rangle.$$

Rearranging the equation we see:

$$\frac{\partial E}{\partial\lambda} = \left\langle\frac{\partial\Psi}{\partial\lambda}\middle|\hat{H}\middle|\Psi\right\rangle - E\left\langle\frac{\partial\Psi}{\partial\lambda}\middle|\Psi\right\rangle + \left\langle\Psi\middle|\frac{\partial\hat{H}}{\partial\lambda}\middle|\Psi\right\rangle + \left\langle\Psi\middle|\hat{H}\middle|\frac{\partial\Psi}{\partial\lambda}\right\rangle - E\left\langle\Psi\middle|\frac{\partial\Psi}{\partial\lambda}\right\rangle.$$

and recalling that if we have a Hermitian Hamiltonian (which we do because the Hamiltonian is equal to its Hermitian conjugate: $\hat{H} = \hat{H}^\dagger$ where $\hat{H}^\dagger \equiv \widetilde{\hat{H}^*}$; the complex conjugate of the transpose of $\hat{H}$ [7]) the Schrödinger equation gives $\hat{H}|\Psi\rangle = E|\Psi\rangle$ and $\langle\Psi|\hat{H} = \langle\Psi|E$. So therefore:

$$\left\langle\frac{\partial\Psi}{\partial\lambda}\middle|\hat{H}\middle|\Psi\right\rangle = E\left\langle\frac{\partial\Psi}{\partial\lambda}\middle|\Psi\right\rangle \text{ and } \left\langle\Psi\middle|\hat{H}\middle|\frac{\partial\Psi}{\partial\lambda}\right\rangle = E\left\langle\Psi\middle|\frac{\partial\Psi}{\partial\lambda}\right\rangle$$

and thus:

$$\frac{\partial E}{\partial\lambda} = \left\langle\Psi\middle|\frac{\partial\hat{H}}{\partial\lambda}\middle|\Psi\right\rangle.$$

Appendix B:

CALCULATING THE SERIES EXPANSION FOR THE ENERGY

In this appendix, I use both the Hypervirial and Hellmann-Feynman Theorems to determine the coefficients, $E_n^{(i)}$, in the expansion of the energy. Before this can be accomplished, we need these commutator ($[\Lambda,\Theta] = \Lambda\Theta - \Theta\Lambda$) relations from Quantum Mechanics:

$$\begin{aligned}
[p, x^r] &= -irx^{r-1} \\
&\quad \Rightarrow \langle\Psi|\left(px^r - x^r p\right)|\Psi\rangle = \langle\Psi| -irx^{r-1}|\Psi\rangle \\
&\quad \Rightarrow \langle\Psi|\left(px^r\right)|\Psi\rangle = \langle\Psi| -irx^{r-1} + x^r p|\Psi\rangle \\
\left[p^2, x^r\right] &= -2irx^{r-1}p - r(r-1)x^{r-2} \\
&\quad \Rightarrow \langle\Psi|\left(p^2x^r - x^r p^2\right)|\Psi\rangle = \langle\Psi| -2irx^{r-1}p - r(r-1)x^{r-2}|\Psi\rangle \\
&\quad \Rightarrow \langle\Psi|\left(p^2x^r\right)|\Psi\rangle = \langle\Psi| -2irx^{r-1}p - r(r-1)x^{r-2} + x^r p^2|\Psi\rangle \\
\left[p^3, x^r\right] &= -3irx^{r-1}p^2 - 3r(r-1)x^{r-2}p + ir(r-1)(r-2)x^{r-3} \\
&\quad \Rightarrow \langle\Psi|\left(p^3x^r - x^r p^3\right)|\Psi\rangle = \langle\Psi| -3irx^{r-1}p^2 - 3r(r-1)x^{r-2}p + ir(r-1)(r-2)x^{r-3}|\Psi\rangle \\
&\quad \Rightarrow \langle\Psi|\left(p^3x^r\right)|\Psi\rangle = \langle\Psi| -3irx^{r-1}p^2 - 3r(r-1)x^{r-2}p + ir(r-1)(r-2)x^{r-3} + x^r p^3|\Psi\rangle
\end{aligned}$$

These commutator relations are easily derived. Consider a generic test function, f_x, and apply the definition of the commutator:

$$\begin{aligned}
[p, x^r]\, f_x &= px^r f_x - x^r p f_x \text{ but } p \equiv \tfrac{\hbar}{i}\tfrac{d}{dx} \\
&= \frac{\hbar}{i}\frac{d}{dx}(x^r f_x) - x^r \frac{\hbar}{i}\frac{df_x}{dx} \text{ and applying the Chain Rule to the first term} \\
&= \frac{\hbar}{i} r x^{r-1} f_x + x^r \frac{\hbar}{i}\frac{df_x}{dx} - x^r \frac{\hbar}{i}\frac{df_x}{dx} \\
&= \frac{\hbar}{i} r x^{r-1} f_x \text{ and in this paper we let } \hbar = 1 \\
&= -irx^{r-1} f_x
\end{aligned}$$

Therefore, $[p, x^r] = -irx^{r-1}$ and the other two commutator relations follow similarly by using the definitions $p^2 \equiv \frac{\hbar}{i}\frac{d^2}{dx^2}$ and $p^3 \equiv \frac{\hbar}{i}\frac{d^3}{dx^3}$.

Finding Recurrence Relations. We are given a Hamiltonian describing the anharmonic oscillator by the potential $V(x) = \frac{1}{2}\omega^2 x^2 + \frac{1}{2}\lambda x^2 + \lambda^2 x^3$:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) = \frac{\hbar^2}{2m}\hat{p}^2 + V(x).$$

and we want to find the coefficients of the energies. A similar problem was discussed in a paper by Altuğ Arda [9] where this problem is solved in a similar manner as follows, however, the paper stops short of finding the entire recurrence relation. We can do better:

From the Schrödinger equation we have:

$$\langle\Psi|\hat{H} = \langle\Psi|E$$

substituting in for $\hat{H}$:

$$\langle\Psi|\left(\frac{1}{2}\hat{p}^2+\frac{1}{2}\omega^2x^2+\frac{1}{2}\lambda x^2+\lambda^2x^3\right)=\langle\Psi|E$$

and solving for $\langle\Psi|\hat{p}^2$:

$$\begin{aligned}\langle\Psi|\left(\frac{1}{2}\hat{p}^2\right) &= \langle\Psi|\left(E-\frac{1}{2}\omega^2x^2-\frac{1}{2}\lambda x^2-\lambda^2x^3\right)\\ \langle\Psi|\hat{p}^2 &= \langle\Psi|\left(2E-\omega^2x^2-\lambda x^2-2\lambda^2x^3\right)\end{aligned}$$

Now expanding the Hypervirial Theorem:

$$\begin{aligned}0 &= \left\langle\Psi\middle|\left[\hat{H},\hat{p}\hat{x}^r\right]\middle|\Psi\right\rangle\\ &= \left\langle\Psi\middle|\left(\hat{H}\hat{p}\hat{x}^r-\hat{p}\hat{x}^r\hat{H}\right)\middle|\Psi\right\rangle\\ &= \left\langle\Psi\middle|\hat{H}\hat{p}\hat{x}^r\middle|\Psi\right\rangle-\left\langle\Psi\middle|\hat{p}\hat{x}^r\hat{H}\middle|\Psi\right\rangle\end{aligned}$$

And combining it with what was found from the Schrödinger equation:

$$\begin{aligned}0 &= \left\langle\Psi\middle|\hat{H}\hat{p}\hat{x}^r\middle|\Psi\right\rangle-\left\langle\Psi\middle|\hat{p}\hat{x}^r\hat{H}\middle|\Psi\right\rangle\\ &= \left\langle\Psi\middle|\left(\frac{1}{2}\hat{p}^2+\frac{1}{2}\omega^2\hat{x}^2+\frac{1}{2}\lambda\hat{x}^2+\lambda^2\hat{x}^3\right)\hat{p}\hat{x}^r\middle|\Psi\right\rangle\\ &\qquad -\left\langle\Psi\middle|\hat{p}\hat{x}^r\left(\frac{1}{2}\hat{p}^2+\frac{1}{2}\omega^2\hat{x}^2+\frac{1}{2}\lambda\hat{x}^2+\lambda^2\hat{x}^3\right)\middle|\Psi\right\rangle\\ &= \left\langle\Psi\middle|\left(\frac{1}{2}\hat{p}^3\hat{x}^r+\frac{1}{2}\omega^2\hat{x}^2\hat{p}\hat{x}^r+\frac{1}{2}\lambda\hat{x}^2\hat{p}\hat{x}^r+\lambda^2\hat{x}^3\hat{p}\hat{x}^r\right)\middle|\Psi\right\rangle\\ &\qquad -\left\langle\Psi\middle|\left(\hat{p}\hat{x}^r\frac{1}{2}\hat{p}^2+\hat{p}\hat{x}^r\frac{1}{2}\omega^2\hat{x}^2+\hat{p}\hat{x}^r\frac{1}{2}\lambda\hat{x}^2+\hat{p}\hat{x}^r\lambda^2\hat{x}^3\right)\middle|\Psi\right\rangle\\ &= \left\langle\Psi\middle|\left(\frac{1}{2}\hat{p}^3\hat{x}^r+\frac{1}{2}\omega^2\hat{x}^2\hat{p}\hat{x}^r+\frac{1}{2}\lambda\hat{x}^2\hat{p}\hat{x}^r+\lambda^2\hat{x}^3\hat{p}\hat{x}^r-\hat{p}\hat{x}^r\frac{1}{2}\hat{p}^2-\hat{p}\hat{x}^r\frac{1}{2}\omega^2\hat{x}^2-\hat{p}\hat{x}^r\frac{1}{2}\lambda\hat{x}^2-\hat{p}\hat{x}^r\lambda^2\hat{x}^3\right)\middle|\Psi\right\rangle\end{aligned}$$

Using the commutator relations we get:

$$\begin{aligned}0 = \Big\langle\Psi\Big|&\frac{1}{2}\left(-3ir\hat{x}^{r-1}\hat{p}^2-3r(r-1)\hat{x}^{r-2}\hat{p}+ir(r-1)(r-2)\hat{x}^{r-3}+\hat{x}^r\hat{p}^3\right)+\frac{1}{2}\omega^2\hat{x}^2\left(-ir\hat{x}^{r-1}+\hat{x}^r\hat{p}\right)\\ &+\frac{1}{2}\lambda\hat{x}^2\left(-ir\hat{x}^{r-1}+\hat{x}^r\hat{p}\right)+\lambda^2\hat{x}^3\left(-ir\hat{x}^{r-1}+\hat{x}^r\hat{p}\right)+\left(ir\hat{x}^{r-1}-\hat{x}^r\hat{p}\right)\frac{1}{2}\hat{p}^2\\ &+\left(ir\hat{x}^{r-1}-\hat{x}^r\hat{p}\right)\frac{1}{2}\omega^2\hat{x}^2+\left(ir\hat{x}^{r-1}-\hat{x}^r\hat{p}\right)\frac{1}{2}\lambda\hat{x}^2+\left(ir\hat{x}^{r-1}-\hat{x}^r\hat{p}\right)\lambda^2\hat{x}^3\Big|\Psi\Big\rangle\end{aligned}$$

Expanding the parentheses and simplifying the expression by cancelling like terms yields:

$$\begin{aligned}
0 &= \left\langle\Psi\right| -\frac{3}{2}ir\hat{x}^{r-1}\hat{p}^2 - \frac{3}{2}r(r-1)\hat{x}^{r-2}\hat{p} + \frac{1}{2}ir(r-1)(r-2)\hat{x}^{r-3} + \frac{1}{2}\omega^2\hat{x}^{r+2}\hat{p} \\
&\quad + \frac{1}{2}\lambda\hat{x}^{r+2}\hat{p} + \lambda^2\hat{x}^{r+3}\hat{p} + \frac{1}{2}ir\hat{x}^{r-1}\hat{p}^2 - \frac{1}{2}\omega^2\hat{x}^r\hat{p}\hat{x}^2 - \frac{1}{2}\lambda\hat{x}^r\hat{p}\hat{x}^2 - \lambda^2\hat{x}^r\hat{p}\hat{x}^3\left|\Psi\right\rangle \\
&= \left\langle\Psi\right| -ir\hat{x}^{r-1}\hat{p}^2 - \frac{3}{2}r(r-1)\hat{x}^{r-2}\hat{p} + \frac{1}{2}ir(r-1)(r-2)\hat{x}^{r-3} + \frac{1}{2}\omega^2\hat{x}^{r+2}\hat{p} \\
&\quad + \frac{1}{2}\lambda\hat{x}^{r+2}\hat{p} + \lambda^2\hat{x}^{r+3}\hat{p} - \frac{1}{2}\omega^2\hat{x}^r\hat{p}\hat{x}^2 - \frac{1}{2}\lambda\hat{x}^r\hat{p}\hat{x}^2 - \lambda^2\hat{x}^r\hat{p}\hat{x}^3\left|\Psi\right\rangle
\end{aligned}$$

Again, using the commutator relations and cancelling like terms:

$$\begin{aligned}
0 &= \left\langle\Psi\right| -ir\hat{x}^{r-1}\hat{p}^2 - \frac{3}{2}r(r-1)\hat{x}^{r-2}\hat{p} + \frac{1}{2}ir(r-1)(r-2)\hat{x}^{r-3} + \frac{1}{2}\omega^2\hat{x}^{r+2}\hat{p} + \frac{1}{2}\lambda\hat{x}^{r+2}\hat{p} \\
&\quad + \lambda^2\hat{x}^{r+3}\hat{p} - \frac{1}{2}\omega^2\hat{x}^r\left(-2i\hat{x} + \hat{x}^2\hat{p}\right) - \frac{1}{2}\lambda\hat{x}^r\left(-2i\hat{x} + \hat{x}^2\hat{p}\right) - \lambda^2\hat{x}^r\left(-3i\hat{x}^2 + \hat{x}^3\hat{p}\right)\left|\Psi\right\rangle \\
&= \left\langle\Psi\right| -ir\hat{x}^{r-1}\hat{p}^2 - \frac{3}{2}r(r-1)\hat{x}^{r-2}\hat{p} + \frac{1}{2}ir(r-1)(r-2)\hat{x}^{r-3} + i\omega^2\hat{x}^{r+1} + i\lambda\hat{x}^{r+1} + 3i\lambda^2\hat{x}^{r+2}\left|\Psi\right\rangle
\end{aligned}$$

Also, if we allow $\hat{O} = \hat{x}^r$ we get $\langle\Psi|\hat{x}^{r-2}\hat{p}|\Psi\rangle = \frac{i}{2}(r-2)\langle\Psi|\hat{x}^{r-3}|\Psi\rangle$ from the Hypervirial Theorem. Thus, we have:

$$\begin{aligned}
0 &= \left\langle\Psi\right| -ir\hat{x}^{r-1}\hat{p}^2 - \frac{3}{4}ir(r-1)(r-2)\hat{x}^{r-3} + \frac{1}{2}ir(r-1)(r-2)\hat{x}^{r-3} + i\omega^2\hat{x}^{r+1} + i\lambda\hat{x}^{r+1} + 3i\lambda^2\hat{x}^{r+2}\left|\Psi\right\rangle \\
&= \left\langle\Psi\right| -ir\hat{x}^{r-1}\hat{p}^2 - \frac{3}{4}ir(r-1)(r-2)\hat{x}^{r-3} + \frac{1}{2}ir(r-1)(r-2)\hat{x}^{r-3} + i\omega^2\hat{x}^{r+1} + i\lambda\hat{x}^{r+1} + 3i\lambda^2\hat{x}^{r+2}\left|\Psi\right\rangle \\
&= \left\langle\Psi\right| -ir\hat{x}^{r-1}\hat{p}^2 - \frac{1}{4}ir(r-1)(r-2)\hat{x}^{r-3} + i\omega^2\hat{x}^{r+1} + i\lambda\hat{x}^{r+1} + 3i\lambda^2\hat{x}^{r+2}\left|\Psi\right\rangle
\end{aligned}$$

From the Schrödinger equation: $\hat{p}^2|\Psi\rangle = (2E - \omega^2\hat{x}^2 - \lambda\hat{x}^2 - 2\lambda^2\hat{x}^3)|\Psi\rangle$ so :

$$\begin{aligned}
0 &= \left\langle\Psi\right| -ir\hat{x}^{r-1}\left(2E - \omega^2\hat{x}^2 - \lambda\hat{x}^2 - 2\lambda^2\hat{x}^3\right) - \frac{1}{4}ir(r-1)(r-2)\hat{x}^{r-3} + i\omega^2\hat{x}^{r+1} + i\lambda\hat{x}^{r+1} + 3i\lambda^2\hat{x}^{r+2}\left|\Psi\right\rangle \\
&= \left\langle\Psi\right| -2ir\hat{x}^{r-1}E + \left[i\omega^2(r+1) + i\lambda(r+1)\right]\hat{x}^{r+1} + (3+2r)i\lambda^2\hat{x}^{r+2} - \frac{1}{4}ir(r-1)(r-2)\hat{x}^{r-3}\left|\Psi\right\rangle \\
&= \left\langle\Psi\right| -2ir\hat{x}^{r-1}E + i(\lambda+\omega^2)(r+1)\hat{x}^{r+1} + i\lambda^2(3+2r)\hat{x}^{r+2} - \frac{1}{4}ir(r-1)(r-2)\hat{x}^{r-3}\left|\Psi\right\rangle
\end{aligned}$$

Moving the term with the Energy to the left hand side:

$$\begin{aligned}
E\left\langle\Psi\middle|\hat{x}^{r-1}\middle|\Psi\right\rangle &= \left\langle\Psi\right|\frac{1}{2ir}\left[i(\lambda+\omega^2)(r+1)\hat{x}^{r+1} + i\lambda^2(3+2r)\hat{x}^{r+2} - \frac{1}{4}ir(r-1)(r-2)\hat{x}^{r-3}\right]\left|\Psi\right\rangle \\
&= \left\langle\Psi\right|(\lambda+\omega^2)\frac{(r+1)}{2r}\hat{x}^{r+1} + \lambda^2\frac{(3+2r)}{2r}\hat{x}^{r+2} - \frac{r(r-1)(r-2)}{8r}\hat{x}^{r-3}\left|\Psi\right\rangle
\end{aligned}$$

Now, let $N = r - 1$:

$$\begin{aligned} E\left\langle \Psi \middle| \hat{x}^N \middle| \Psi \right\rangle &= \left\langle \Psi \middle| (\lambda+\omega^2)\frac{(N+2)}{2(N+1)}\hat{x}^{N+2} + \lambda^2\frac{(3+2(N+1))}{2(N+1)}\hat{x}^{N+3} - \frac{(N+1)N(N-1)}{8(N+1)}\hat{x}^{N-2} \middle| \Psi \right\rangle \\ &= \left\langle \Psi \middle| (\lambda+\omega^2)\frac{(N+2)}{2(N+1)}\hat{x}^{N+2} + \lambda^2\frac{(2N+5)}{2(N+1)}\hat{x}^{N+3} - \frac{1}{8}N(N-1)\hat{x}^{N-2} \middle| \Psi \right\rangle \end{aligned}$$

Therefore,

$$E\left\langle \Psi | x^N | \Psi \right\rangle = (\lambda+\omega^2)\frac{N+2}{2(N+1)}\left\langle \Psi | x^{N+2} | \Psi \right\rangle + \lambda^2\frac{2N+5}{2(N+1)}\left\langle \Psi | x^{N+3} | \Psi \right\rangle - \frac{1}{8}N(N-1)\left\langle \Psi | x^{N-2} | \Psi \right\rangle \tag{4}$$

which is Eq. (3) in Arda [9].

Assume the following power series expansions:

$$E = \sum_{k=0}^{\infty} E_n^{(k)}\lambda^k$$

$$\langle \Psi | x^s | \Psi \rangle = \sum_{k=0}^{\infty} A_s^{(k)}\lambda^k$$

Notice that when $s = 1$ we get the equality $1 = \sum_{k=0}^{\infty} A_s^{(k)}\lambda^k$ and if we let $A_0^{(0)} = 1$ then $A_0^{(k)}$ must equal 0 for all k. Also, for $k = 0$ we get $E = E_n^{(0)}$ which is the energy associated with the harmonic oscillator [7]:

$$E_n^{(0)} = \hbar\omega\left(n + \frac{1}{2}\right)$$

Substituting these power series expansions into Eq. (4) we find:

$$\begin{aligned} &\left(\sum_{k=0}^{\infty} E_n^{(k)}\lambda^k\right)\left(\sum_{k=0}^{\infty} A_N^{(k)}\lambda^k\right) \\ =\ & (\lambda+\omega^2)\frac{N+2}{2(N+1)}\sum_{k=0}^{\infty} A_{N+2}^{(k)}\lambda^k + \lambda^2\frac{2N+5}{2(N+1)}\sum_{k=0}^{\infty} A_{N+3}^{(k)}\lambda^k - \frac{1}{8}N(N-1)\sum_{k=0}^{\infty} A_{N-2}^{(k)}\lambda^k \\ =\ & \sum_{k=0}^{\infty}\left[(\lambda+\omega^2)\frac{N+2}{2(N+1)}A_{N+2}^{(k)}\lambda^k + \lambda^2\frac{2N+5}{2(N+1)}A_{N+3}^{(k)}\lambda^k - \frac{1}{8}N(N-1)A_{N-2}^{(k)}\lambda^k\right] \\ =\ & \sum_{k=0}^{\infty}\left[\frac{2N+5}{2(N+1)}A_{N+3}^{(k)}\lambda^{k+2} + \frac{N+2}{2(N+1)}A_{N+2}^{(k)}\lambda^{k+1} + \left(\frac{N+2}{2(N+1)}\omega^2 A_{N+2}^{(k)} - \frac{1}{8}N(N-1)A_{N-2}^{(k)}\right)\lambda^k\right] \end{aligned} \tag{5}$$

Now, consider the left hand side. Examining the form of the product of two infinite sums [2] we have:

$$\left[\sum_{n=0}^{\infty} a_n(x-x_0)^n\right]\left[\sum_{n=0}^{\infty} b_n(x-x_0)^n\right] = \sum_{n=0}^{\infty} c_n(x-x_0)^n$$

where

$$c_n = a_0 b_n + a_1 b_{n-1} + \cdots + a_n b_0 = \sum_{i=0}^{n} a_i b_{n-1}$$

then the left hand side of Eq. (5) reads:

$$\left(\sum_{k=0}^{\infty} E_n^{(k)} \lambda^k\right)\left(\sum_{k=0}^{\infty} A_N^{(k)} \lambda^k\right) = \sum_{k=0}^{\infty} c_k \lambda^k$$

where

$$c_k = \sum_{i=0}^{k} E_n^i A_N^{k-i}$$

so then we have

$$\sum_{k=0}^{\infty} c_k \lambda^k = \sum_{k=0}^{\infty} \left[\frac{2N+5}{2(N+1)} A_{N+3}^{(k)} \lambda^{k+2} + \frac{N+2}{2(N+1)} A_{N+2}^{(k)} \lambda^{k+1} + \left(\frac{N+2}{2(N+1)} \omega^2 A_{N+2}^{(k)} - \frac{1}{8} N(N-1) A_{N-2}^{(k)}\right) \lambda^k\right]$$

Now, separating the sums and pulling out various parameters:

$$\begin{aligned}
& c_0 \lambda^0 + c_1 \lambda^1 + \sum_{k=2}^{\infty} c_k \lambda^k \\
= & \sum_{k=0}^{\infty} \left(\frac{2N+5}{2(N+1)} A_{N+3}^{(k)} \lambda^{k+2}\right) + \sum_{k=0}^{\infty} \left(\frac{N+2}{2(N+1)} A_{N+2}^{(k)} \lambda^{k+1}\right) \\
& \quad + \sum_{k=0}^{\infty} \left(\left(\frac{N+2}{2(N+1)} \omega^2 A_{N+2}^{(k)} - \frac{1}{8} N(N-1) A_{N-2}^{(k)}\right) \lambda^k\right) \\
= & \sum_{k=2}^{\infty} \left(\frac{2N+5}{2(N+1)} A_{N+3}^{(k-2)} \lambda^k\right) + \frac{N+2}{2(N+1)} A_{N+2}^{(0)} \lambda^1 + \sum_{k=2}^{\infty} \left(\frac{N+2}{2(N+1)} A_{N+2}^{(k-1)} \lambda^k\right) \\
& \quad + \left(\frac{N+2}{2(N+1)} \omega^2 A_{N+2}^{(0)} - \frac{1}{8} N(N-1) A_{N-2}^{(0)}\right) \lambda^0 + \left(\frac{N+2}{2(N+1)} \omega^2 A_{N+2}^{(1)} - \frac{1}{8} N(N-1) A_{N-2}^{(1)}\right) \lambda^1 \\
& \quad + \sum_{k=2}^{\infty} \left(\left(\frac{N+2}{2(N+1)} \omega^2 A_{N+2}^{(k)} - \frac{1}{8} N(N-1) A_{N-2}^{(k)}\right) \lambda^k\right)
\end{aligned}$$

collect powers of λ:

$$\begin{aligned}
0 = & \left(\frac{N+2}{2(N+1)} \omega^2 A_{N+2}^{(0)} - \frac{1}{8} N(N-1) A_{N-2}^{(0)} - c_0\right) \lambda^0 \\
& + \left(\frac{N+2}{2(N+1)} A_{N+2}^{(0)} + \frac{N+2}{2(N+1)} \omega^2 A_{N+2}^{(1)} - \frac{1}{8} N(N-1) A_{N-2}^{(1)} - c_1\right) \lambda^1 \\
& + \sum_{k=2}^{\infty} \Big[\Big(\frac{2N+5}{2(N+1)} A_{N+3}^{(k-2)} + \frac{N+2}{2(N+1)} A_{N+2}^{(k-1)} \\
& \qquad + \frac{N+2}{2(N+1)} \omega^2 A_{N+2}^{(k)} - \frac{1}{8} N(N-1) A_{N-2}^{(k)} - c_k\Big) \lambda^k\Big]
\end{aligned}$$

For this to be true, all the coefficients of powers of λ must equal 0:

$$\begin{aligned}
0 &= \frac{N+2}{2(N+1)}\omega^2 A_{N+2}^{(0)} - \frac{1}{8}N(N-1)A_{N-2}^{(0)} - c_0 \\
0 &= \frac{N+2}{2(N+1)}A_{N+2}^{(0)} + \frac{N+2}{2(N+1)}\omega^2 A_{N+2}^{(1)} - \frac{1}{8}N(N-1)A_{N-2}^{(1)} - c_1 \\
0 &= \frac{2N+5}{2(N+1)}A_{N+3}^{(k-2)} + \frac{N+2}{2(N+1)}A_{N+2}^{(k-1)} + \frac{N+2}{2(N+1)}\omega^2 A_{N+2}^{(k)} - \frac{1}{8}N(N-1)A_{N-2}^{(k)} - c_k \text{ for } k = 2,3,4,\ldots
\end{aligned}$$

Substituting in for c_k:

$$0 = \frac{N+2}{2(N+1)}\omega^2 A_{N+2}^{(0)} - \frac{1}{8}N(N-1)A_{N-2}^{(0)} - E_n^{(0)}A_N^{(0)} \tag{6}$$

$$0 = \frac{N+2}{2(N+1)}A_{N+2}^{(0)} + \frac{N+2}{2(N+1)}\omega^2 A_{N+2}^{(1)} - \frac{1}{8}N(N-1)A_{N-2}^{(1)} - E_n^{(0)}A_N^{(1)} - E_n^{(1)}A_N^{(0)} \tag{7}$$

$$\begin{aligned}
0 = {} & \frac{2N+5}{2(N+1)}A_{N+3}^{(k-2)} + \frac{N+2}{2(N+1)}A_{N+2}^{(k-1)} + \frac{N+2}{2(N+1)}\omega^2 A_{N+2}^{(k)} \\
& -\frac{1}{8}N(N-1)A_{N-2}^{(k)} - \sum_{i=0}^{k} E_n^{(i)}A_N^{(k-i)} \text{ for } k = 2,3,4,\ldots
\end{aligned} \tag{8}$$

Solving each equation for $A_N^{(i)}$:

$$\begin{aligned}
A_N^{(0)} &= \frac{1}{E_n^0}\left[\frac{N+2}{2(N+1)}\omega^2 A_{N+2}^{(0)} - \frac{1}{8}N(N-1)A_{N-2}^{(0)}\right] \\
A_N^{(1)} &= \frac{1}{E_n^0}\left[\frac{N+2}{2(N+1)}A_{N+2}^{(0)} + \frac{N+2}{2(N+1)}\omega^2 A_{N+2}^{(1)} - \frac{1}{8}N(N-1)A_{N-2}^{(1)} - E_n^{(1)}A_N^{(0)}\right]
\end{aligned}$$

which are Eqs. (10) and (11) in Arda [9]. If we let $k = 2$ we get Eq.(12) in Arda [9]:

$$\begin{aligned}
A_N^{(2)} = \frac{1}{E_n^{(0)}}\Big[& \frac{N+2}{2(N+1)}\omega^2 A_{N+2}^{(2)} + \frac{N+2}{2(N+1)}A_{N+2}^{(1)} + \frac{2N+5}{2(N+1)}A_{N+3}^{(0)} \\
& -\frac{1}{8}N(N-1)A_{N-2}^{(2)} - E_n^{(1)}A_N^{(1)} - E_n^{(2)}A_N^{(0)}\Big]
\end{aligned}$$

Continuing with the derivation it is possible to calculate recurrence relations for all k (instead of only for $k = 0,1,2$ as done in Arda [9]). Rearranging Eq. (6), (7), and (8) we find:

$$A_{N+2}^{(0)} = \frac{2(N+1)}{N+2}\frac{1}{\omega^2}\left[\frac{1}{8}N(N-1)A_{N-2}^{(0)} + E_n^{(0)}A_N^{(0)}\right]$$

$$A_{N+2}^{(1)} = \frac{2(N+1)}{N+2}\frac{1}{\omega^2}\left[-\frac{N+2}{2(N+1)}A_{N+2}^{(0)} + \frac{1}{8}N(N-1)A_{N-2}^{(1)} + E_n^{(0)}A_N^{(1)} + E_n^{(1)}A_N^{(0)}\right]$$

$$A_{N+2}^{(k)} = \frac{2(N+1)}{N+2}\frac{1}{\omega^2}\left[-\frac{2N+5}{2(N+1)}A_{N+3}^{(k-2)} - \frac{N+2}{2(N+1)}A_{N+2}^{(k-1)} + \frac{1}{8}N(N-1)A_{N-2}^{(k)} + \sum_{i=0}^{k} E_n^{(i)}A_N^{(k-i)}\right] \text{ for } k = 2,3,4,\ldots$$

The three above equations combine to form part of the recurrence relations used to calculate the energies $E_n^{(k)}$.

Now, from the Hellmann-Feynman Theorem:

$$\left\langle \Psi \middle| \frac{\partial V}{\partial \lambda} \middle| \Psi \right\rangle = \frac{\partial E}{\partial \lambda} = \left\langle \Psi \middle| \frac{\partial \hat{H}}{\partial \lambda} \middle| \Psi \right\rangle$$

we can find the remaining necessary recurrence relation. We know:

$$\begin{aligned} \frac{\partial E}{\partial \lambda} &= \frac{\partial}{\partial \lambda}\left[\sum_{k=0}^{\infty} E_n^{(k)} \lambda^k\right] \\ &= \sum_{k=0}^{\infty} E_n^{(k)} \frac{\partial}{\partial \lambda} \lambda^k \\ &= \sum_{k=0}^{\infty} k E_n^{(k)} \lambda^{k-1} \end{aligned}$$

and

$$\begin{aligned} \left\langle \Psi \middle| \frac{\partial \hat{H}}{\partial \lambda} \middle| \Psi \right\rangle &= \left\langle \Psi \middle| \frac{\partial}{\partial \lambda}\left(-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}\omega^2 x^2 + \frac{1}{2}\lambda x^2 + \lambda^2 x^3\right) \middle| \Psi \right\rangle \\ &= \left\langle \Psi \middle| \frac{1}{2}x^2 + 2\lambda x^3 \middle| \Psi \right\rangle \\ &= \sum_{k=0}^{\infty} \frac{1}{2} A_2^{(k)} \lambda^k + \sum_{k=0}^{\infty} 2 A_3^{(k)} \lambda^{k+1}. \end{aligned}$$

Therefore,

$$\begin{aligned} \sum_{k=0}^{\infty} k E_n^{(k)} \lambda^{k-1} &= \sum_{k=0}^{\infty} \frac{1}{2} A_2^{(k)} \lambda^k + \sum_{k=0}^{\infty} 2 A_3^{(k)} \lambda^{k+1} \\ \sum_{k=-1}^{\infty} (k+1) E_n^{(k+1)} \lambda^k - \sum_{k=0}^{\infty} \frac{1}{2} A_2^{(k)} \lambda^k - \sum_{k=1}^{\infty} 2 A_3^{(k-1)} \lambda^k &= 0 \\ 0 E_n^{(0)} \lambda^{-1} + E_n^{(1)} \lambda^0 - \frac{1}{2} A_2^{(0)} \lambda^0 + \sum_{k=1}^{\infty}\left((k+1) E_n^{(k+1)} - \frac{1}{2} A_2^{(k)} - 2 A_3^{(k-1)}\right) \lambda^k &= 0. \end{aligned}$$

Notice that $E_n^{(1)} - \frac{1}{2}A_2^{(0)}$ and $(k+1)E_n^{(k+1)} - \frac{1}{2}A_2^{(k)} - 2A_3^{(k-1)}$ must equal 0 for all values of λ:

$$\begin{aligned} E_n^{(1)} - \frac{1}{2} A_2^{(0)} &= 0 \\ \Rightarrow E_n^{(1)} &= \frac{1}{2} A_2^{(0)} \\ (k+1) E_n^{(k+1)} - \frac{1}{2} A_2^{(k)} - 2 A_3^{(k-1)} &= 0 \text{ for } k = 1, 2, 3, \ldots \\ \Rightarrow E_n^{(k+1)} &= \frac{1}{2(k+1)} A_2^{(k)} + \frac{2}{(k+1)} A_3^{(k-1)} \text{ for } k = 1, 2, 3, \ldots \end{aligned}$$

which is Eq. (9) in Arda [9].

The set of recursion equations are now:

$$\begin{aligned}
A_{N+2}^{(0)} &= \frac{2(N+1)}{N+2}\frac{1}{\omega^2}\left[\frac{1}{8}N(N-1)A_{N-2}^{(0)}+E_n^{(0)}A_N^{(0)}\right] \\
A_{N+2}^{(1)} &= \frac{2(N+1)}{N+2}\frac{1}{\omega^2}\left[-\frac{N+2}{2(N+1)}A_{N+2}^{(0)}+\frac{1}{8}N(N-1)A_{N-2}^{(1)}+E_n^{(0)}A_N^{(1)}+E_n^{(1)}A_N^{(0)}\right] \\
A_{N+2}^{(k)} &= \frac{2(N+1)}{N+2}\frac{1}{\omega^2} \\
&\qquad \left[-\frac{2N+5}{2(N+1)}A_{N+3}^{(k-2)}-\frac{N+2}{2(N+1)}A_{N+2}^{(k-1)}+\frac{1}{8}N(N-1)A_{N-2}^{(k)}+\sum_{i=0}^{k}E_n^{(i)}A_N^{(k-i)}\right] \text{ for } k=2,3,4,\ldots \\
E_n^{(0)} &= \hbar\omega\left(n+\frac{1}{2}\right) \\
E_n^{(1)} &= \frac{1}{2}A_2^{(0)} \\
E_n^{(k+1)} &= \frac{1}{2(k+1)}A_2^{(k)}+\frac{2}{(k+1)}A_3^{(k-1)} \text{ for } k=1,2,3,\ldots
\end{aligned}$$

Now let $s=N+2$ and $r=k+1$ and adjust the indices of the $A_s^{(r-1)}$ term:

$$\begin{aligned}
A_s^{(0)} &= \frac{2(s-1)}{s}\frac{1}{\omega^2}\left[\frac{1}{8}(s-2)(s-3)A_{s-4}^{(0)}+E_n^{(0)}A_{s-2}^{(0)}\right] \\
A_s^{(1)} &= \frac{2(s-1)}{s}\frac{1}{\omega^2}\left[-\frac{s}{2(s-1)}A_s^{(0)}+\frac{1}{8}(s-2)(s-3)A_{s-4}^{(1)}+E_n^{(0)}A_{s-2}^{(1)}+E_n^{(1)}A_{s-2}^{(0)}\right] \\
A_s^{(r)} &= \frac{2(s-1)}{s}\frac{1}{\omega^2} \\
&\qquad \left[-\frac{2s+1}{2(s-1)}A_{s+1}^{(r-2)}-\frac{s}{2(s-1)}A_s^{(r-1)}+\frac{1}{8}(s-2)(s-3)A_{s-4}^{(r)}+\sum_{i=0}^{r}E_n^{(i)}A_{s-2}^{(r-i)}\right] \text{ for } r=2,3,4,\ldots \\
E_n^{(0)} &= \hbar\omega\left(n+\frac{1}{2}\right) \\
E_n^{(1)} &= \frac{1}{2}A_2^{(0)} \\
E_n^{(r)} &= \frac{1}{2(r)}A_2^{(r-1)}+\frac{2}{(r)}A_3^{(r-2)} \text{ for } r=2,3,4,\ldots
\end{aligned}$$

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