PADÉ APPROXIMANTS AND THE ANHARMONIC OSCILLATOR

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1 Introduction

Several problems in physics, while in principle having been solved, do not admit closed form solutions. In particular, problems in perturbation theory, where in principle a problem may be solved to all orders in a perturbative parameter with sufficient effort. Padé approximation is a very simple and powerful generalisation of Taylor approximation. This method efficiently extracts quantitative and qualitative information about solutions from formal power series obtained perturbatively. One of the simplest non-trivial cases of this occurs while computing the energy eigenvalue expansion quartic quantum anharmonic oscillator, an oscillator system where the quadratic potential has a small quartic correction:

$$H = p^2 + x^2 + \beta x^4$$

where β is the small parameter in which perturbative expansions are generated.

By analytic continuation, a convergent power series can be used to determine a function everywhere up to a natural boundary (a dense set of singularities). However in practice, this convergence may be impractically slow, or may not converge at all to the point of interest. This can be overcome in certain cases through the theory of Padé approximants.

In chapter 2, we will study the properties of Padé approximants. In chapter 3, we will discuss the anharmonic oscillator, and in chapter 4 we will discuss the application of the Padé approximant method to the physical problem of the quantum anharmonic oscillator.

2 Padé Approximants: Convergence and Analytic Properties

Padé approximants generalise Taylor approximation by using rational functions instead of polynomials. They can be formally defined as follows.

Definition 2.1. The $[N, M]_f$ Padé approximant associated with a formal power series $f(z) = \sum a_n z^n$ is the unique rational function $[N, M]_f(z)$ of degree N in the numerator and degree M in the denominator such that

$$[N, M](z) - \sum_{n=0}^{M+N} a_n z^n = O\big(z^{M+N+1}\big) \tag{1}$$

Note. When f is clear from context, it may be suppressed

$$[M, N] := [M, N]_f$$

The given definition is not a constructive one, and it is in general fairly difficult to construct Padé approximants from this definition. There is however a constructive algorithm to directly compute them. The exact Padé approximant can be computed explicitly using the coefficients of the power series:

$$[M,N](z) = \frac{\begin{vmatrix} a_{M-N+1} & a_{M-N+2} & \dots & a_{M+1} \\ \vdots & \vdots & \ddots & \\ a_M & a_{M+1} & \dots & a_{M+N} \\ \sum_{n=N}^{M} a_{n-N} z^n & \sum_{n=N-1}^{M} a_{n-N+1} z^n & \dots & \sum_{n=0}^{M} a_n z^n \end{vmatrix}}{\begin{vmatrix} a_{M-N+1} & a_{M-N+2} & \dots & a_{M+1} \\ \vdots & \vdots & \ddots & \\ a_M & a_{M+1} & \dots & a_{M+N} \\ z^N & z^{N-1} & \dots & 1 \end{vmatrix}} \tag{2}$$

where $\forall n < 0 \; a_n := 0$.[1]

Theorem 2.1 (Uniqueness)**.** *The rational function obtained from Equation (2) is the unique function satisfying Definition 2.1*

Proof. Let $\frac{P(z)}{Q(z)}$ be any rational function satisfying Definition 1.1. Let

$$[N,M](z) = \frac{R(z)}{S(z)}$$

.

Consider

$$\left\{[N,M](z) - \frac{P(z)}{Q(z)}\right\} Q(z)S(z) \tag{3}$$

. This expression is a degree $M+N$ polynomial, but by Equation (1) this expression is in $O(z^{M+N+1})$, hence this expression is identically zero. Hence

$[N, M](z) = \frac{P(z)}{Q(z)}$ upto cancellation of common factors between the numerator and denominator. $\square$

Just as Taylor polynomials in $\mathbb{C}[z]$ the polynomial ring, can be extended to Taylor series in $\mathbb{C}[[z]]$ the power series ring, Padé approximants in $\mathbb{C}[z, z^{-1}]$ can first be extended to series with infinitely many terms in the numerator and finitely many terms in the denominator or vice versa, in $\mathbb{C}[[z, z^{-1}]$ and $\mathbb{C}[z, z^{-1}]]$ and then further be extended to infinite degree in both the numerator and denominator in $\mathbb{C}[[z, z^{-1}]]$. The former are more amenable to rigorous theorems, but the latter are more powerful and useful when applied to problems in physics.

Theorem 2.2 (de Montessus de Balloire, 1902)**.** *Let $f(z)$ be meromorphic on $|z| \leqslant R$ with m poles. Then*

$$\lim_{N \to \infty} [N, m](z) = f(z)$$

uniformly on $\{|z| \leqslant R\} \backslash \{\epsilon-$disks around the poles$\}$.

This result also holds if the degree of the denominator goes to infinity while the degree of the numerator is kept finite.

Remark. $\forall n \in \mathbb{Z}$ the study of $[N + k, N]$ Padé approximants of a function f can be reduced to the study of $[N, N]$ of a function g related to f as

$$g(z) = \begin{cases} z^{-n} f(z) & n \leqslant 0 \\ z^{-n} \left[f(z) - \sum_{i=0}^{n} a_i z^i \right] & n > 0 \end{cases} \tag{4}$$

where a_i are the Taylor coefficients of f.

2.1 Conformal Structure

The conformal structure preserving transformations of the complex plane are called linear fractional transformations. They are maps of the form

$$z \mapsto \frac{az + b}{cz + d}$$

with $a, b, c, d \in \mathbb{C}, ad - bc \neq 0$. This set of tranformations forms a group $\mathscr{M}$ under composition.

Definition 2.2. The group of **homographic transformations** $\mathscr{H}$ is the subgroup of the group of linear fractional transformations that are of the form

$$z \mapsto \frac{az}{1 + bz}$$

Theorem 2.3.

$$\forall \phi \in \mathscr{H} \quad [N, N]_{f \circ \phi} = [N, N]_f \circ \phi \tag{5}$$

Proof. Let $\phi(z) = \frac{az}{1+bz}$ and $[N, N]_f = \frac{P}{Q}$.

$$[N,N]_f \circ \phi(z) = \frac{P\left(\frac{az}{1+bz}\right)}{Q\left(\frac{az}{1+bz}\right)} \times \frac{(1+bz)^N}{(1+bz)^N} = \frac{p(z)}{q(z)}$$

for some degree N polynomials p, q. Expanding as a power series this agrees term by term to the power series expansions of $f\left(\frac{az}{1+bz}\right)$ at least to order z^{2N}. Hence by the uniqueness theorem of Padé approximants, Theorem 2.1,

$$\frac{p}{q} = \frac{P \circ \phi}{Q \circ \phi} = [N,N]_{f \circ \phi}$$

□

Theorem 2.4.

$$\forall \rho \in \mathscr{M} \quad [N,N]_{\rho \circ f} = \rho \circ [N,N]_f \tag{6}$$

Proof. Let $\rho(z) = \frac{az+b}{cz+d}$ and $[N,N]_f = \frac{P}{Q}$.

$$\rho \circ [N,N]_f(z) = \frac{a\frac{P(z)}{Q(z)} + b}{c\frac{P(z)}{Q(z)} + d} \times \frac{Q(z)}{Q(z)} = \frac{p(z)}{q(z)}$$

degree N polynomials $p = aP + bQ, q = cP + dQ$. Again $\frac{p}{q} = [N,N]_{\rho \circ f}$ by Theorem 2.1 □

Using these theorems, one can prove the following convergence theorem

Theorem 2.5. *Let $\{f_k(z)\}_{k \in \mathbb{N}}$ be a sequence of $[N_k, M_k]$ Padé approximants, such that*

$$\lim_{k \to \infty} N_k + M_k = \infty$$

. Then if $|f_k|$ is uniformly bounded on $\overline{D}_R(0)$ then $\exists r < R$ and $\exists f$ analytic,

such that $f_k(z) \to f(z)$ uniformly on $\overline{D}_r(0)$ and f has a power series with radius convergence $\geqslant R$. [2]

Proof. Let $\epsilon > 0$ be arbitrary. f_k be uniformly bounded by B on $\overline{D}_R(0)$. $f_k = [N_k, M_k]$ rational and bounded on a compact subset of $\mathbb{C} \implies f_k$ is analytic on $\overline{D}_R(0) \implies$ its power series $\sum_n a_k(n)z^n$ had radius of convergence $\geqslant R$. By Cauchy's inequality for the Taylor series coefficients of a complex analytic function $a_k(n)$ is bounded uniformly in k by B/R^n. Hence

$$\left| f_k(z) - \sum_{n=0}^{t} a_k(n)z^n \right| \leqslant \sum_{n=t+1}^{\infty} |a_k(n)z^n| \leqslant \sum_{n=t+1}^{\infty} W\left(\frac{r}{R}\right)^n = \frac{W\left(\frac{r}{R}\right)^{t+1}}{1-\frac{r}{R}} \tag{7}$$

$\frac{r}{R} < 1 \implies$ for sufficiently large t

$$\left| f_k(z) - \sum_{n=0}^{t} a_k(n)z^n \right| < \frac{\epsilon}{2}$$

uniformly in k. $\lim_{k\to\infty} N_k + M_k = \infty \implies \exists K \in \mathbb{N}\ \forall k \geqslant K\ N + M \geqslant t$. Hence by the uniqueness theorem, Theorem 2.1, the first $t+1$ terms are identical $\forall k \geqslant K$.

$$\forall j,k \geqslant K\ \forall z \in \overline{D}_r(0)\ |f_k(z) - f_j(z)| \leqslant \left| f_k(z) - \sum_{n=0}^{t} a_k(n)z^n \right| + \left| f_j(z) - \sum_{n=0}^{t} a_j(n)z^n \right| < \epsilon \tag{8}$$

Hence by the uniform convergence theorem the limit, f is analytic on

$D_R(0)$. Hence by Taylor's theorem its power series has radius of convergence at least R. $\square$

This then allows us to constrain the analyticity of the limit function.

Theorem 2.6. *Let $\{f_k(z)\}_{k\in\mathbb{N}}$ be a sequence of $[N_k, M_k]$ Padé approximants, such that*

$$\lim_{k\to\infty} N_k + M_k = \infty$$

. Let D_1, D_2 by closed simply connected domains such that $0 \in \text{int}\, D_1 \cap \text{int}\, D_2$. Then $|f_k|$ is uniformly bounded on D_1 and if $\frac{1}{|f_k|}$ is uniformly bounded on D_2 then $\exists f$ meromorphic, such that $f_k(z) \to f(z)$ uniformly on $\text{int}\, D_1 \cap \text{int}\, D_2$.

Proof. $\exists R_1$ such that $\overline{D}_{R_1} \subseteq D_1$. So by Theorem 2.5 $\exists f$ analytic on $\overline{D}_{R_1}(0)$ such that the sequence converges to uniformly on $\overline{D}_{R_1}(0)$. By applying Theorem 2.5 on a chain of disks, we can extend f to D_1.

$\dfrac{1}{f_k}$ is an $[M_k, N_k]$ Padé approximant, so the $\left\{\dfrac{1}{f_k}\right\}_{n\in\mathbb{N}}$ also form a sequence that satisfies the hypotheses on D_2. Hence again by application of Theorem 2.5, this sequence converges uniformly to $\frac{1}{f}$ analytic. Since the inverse of an analytic function is meromorphic, f is a meromorphic function that f_1 $\square$

Theorem 2.6 is also practically useful. One considers a domain of interest in the complex plane on which on physical grounds it is known that the function is meromorphic. For instance, it is commmon to consider the neighbourhood of a real interval. From an infinite sequence of $[N, M]$ approximants, select a subsequence which satisfies the hypotheses of Theorem

2.6. Then by Theorem 2.6 one has obtained a sequence of rational functions that uniformly converge to the chosen function.[2]

When M or N remains finite, several results are known, and the main mathematical problem associated with the convergence properties and analyticity of Padé approximants is to establish the existence of such an infinite bounded subsequence when both $M, N \to \infty$.

These results are particularly powerful when applied to Stieltjes series, with Baker's paper [1] providing a particularly detailed treatment of this topic.

3 The Anharmonic Oscillator

One of the simplest quantum Hamiltonians that does not, in general, admit closed form solutions in terms of elementary functions is the quartic oscillator $H = p^2 + x^2 + \beta x^4$. As a canonical test case for any perturbative approach, and because of its relation to ϕ^4 field theories, mathematical physics literature is rich with the study of this system. Barry Simon, in a series of papers proved a set of foundational theorems, that have since been built upon in diverse directions. Here we will review a few results governing the coupling constant analyticity and convergence of the energy eigenvalues of this system, before connecting their study to Padé approximants.

3.1 Introduction

For every $\beta > 0$ the energy levels of the Hamiltonian

$$H = p^2 + x^2 + \beta x^4 \tag{9}$$

are analytic in the neighbourhood of $\beta \in (0, \infty)$. However, Rayleigh-Schödinger perturbation series for this system diverges for every β.

The study of this Hamiltonian is of particular interest to theoretical physics because the methods used are directly relevant to field-theoretic systems of the form

$$\mathscr{L} = \partial_\mu \phi \partial^\mu \phi - m^2 \phi^2 - \beta \phi^4, \tag{10}$$

and can in fact be directly transferred to the field theory case if we insist the the fields be normal ordered. Generalising to non-normal ordered fields is non-trivial, but still promising.

One of the earliest results in the area comes from the famous Bender-Wu paper [7] which describes the three sheet branched structure of the $\beta = 0$ singularity, provides bounds on the Rayleigh-Schrödinger coefficients of $E_0(\beta)$ and conjectures the asymptotic behaviour of the perturbation series coefficients.

In a series of papers, Barry Simon then went on to produce several key results in the field including the detailed structure of the the complex $E_n(\beta)$ plane and a rigorous proof of the Bender-Wu formula, among others. Loeffel, Martin, Simon and Wightman[6] introduced the use of Padé approximants to the field, which allowed for extremely accurate numerical estimates. Graffi, Grecchi and Simon [5] proved the perturbation series for the energy levels of the x^4 oscillator can be obtained using a generalised Borel summation method and Padé approximants.

In subsection 2, we review the background material associated with the study of quartic oscillators. Subsection 3 discusses some key results proven in the aforementioned papers.

3.2 The x^4 Oscillator

For the purposes of this problem, it is instructive to study the more general Hamiltonian

$$H(\alpha, \beta) = p^2 + \alpha x^2 + \beta x^4 \tag{11}$$

with eigenvalues $E_n(\alpha, \beta)$. We can apply a scaling argument to these energy eigenvalues through the scale transformation

$$p \mapsto \lambda p, x \mapsto \frac{x}{\lambda} \implies H(\alpha, \beta) \mapsto \lambda^2 H(\frac{\alpha}{\lambda^2}, \frac{\beta}{\lambda^6}) \tag{12}$$

but because scaling is a unitary transformation, both Hamiltonians have the same energies. In particular, we can transform between x^4 as a pertubation of the x^2 oscillator and x^2 as a perturbation of the x^4 oscillator through

$$E_n(1, \beta) = \beta^{\frac{1}{3}} E_n(\beta^{-\frac{2}{3}}, 1) \tag{13}$$

Hence it is equivalent to study $E_n(\alpha, 1)$ as $\alpha \to \infty$ and $E_n(1, \beta)$ as $\beta \to 0$, so the cube root nature of the singularity follows. This also indicates that $E_n(\alpha, \beta)$ is essentially a complex function of only one variable, and hence allows us to apply single-variable complex analysis techniques.

$$\lim_{\alpha \to 0^+} E_n(\alpha, \beta) = \beta^{\frac{1}{3}} E_n(0, 1) \tag{14}$$

The $\alpha \to 0^+$ limit corresponds to massless field theory models. For any $\alpha_0 > 0$, $E_n(\alpha_0, \beta)$ has infinitely many branch points near $\beta = 0$. As $\alpha \to 0^+$, all the branch points approach 0 and at $\alpha = 0$ they merge into a single branch point at $\beta = 0$.

Simon proves that $E_n(1, \beta)$ has a convergent (strong-coupling) expansion in $\beta^{-\frac{2}{3}}$ convergent for large β[4]. He then proves the following result

Theorem 3.1. *Every analytic continuation of $E_n(\alpha, 1)$ is real on the real axis and on every sheet,* $\operatorname{Im} \alpha > 0 \implies \operatorname{Im} E_n > 0$

These techniques also explain the divergence of the perturbation expansions for E. $E_n(1, \beta)$ is not analytic near $\beta = 0$. Hence $E_n(1, \beta)$ cannot be represented by a convergent Taylor series in any neighbourhood of $\beta = 0$.

3.3 Global Structure of E_n

It is conjectured that that $E_n(\alpha, 1)$ can only have isolated singularities in the finite α plane. On the contrary, assume there is a non-isolated at α_0.

Case I: α_0 is the limit point of isolated singularities. Then $E_n(\alpha, 1)$ goes to infinity as $\alpha \to \alpha_0$ crossing infinity many levels along the way.

Case II: α_0 is the limit point of non-isolated singularities. Then α_0 lies on a natural boundary, so E_n is singular on a whole curve or on a Cantor subset of a curve.

Both cases appear to be unphysical hence the conjecture.

There are two key results in the case of isolated singularities.

Theorem 3.2 (Simon, 1969). *$E_n(\alpha, 1)$ has no poles or essential singularities. Algebraic branch points have no negative powers in their Puiseux series.*

This argument does not exclude logarithmic branch points, but as with natural boundaries, these are conjectured not to exist because they appear to be unphysical. However, Loeffel and Martin [ref] proved that there are no branch points of $E_n(1, \beta)$ of any kind in the region $|\arg \beta| < \pi$.

This leaves us to study the case of the $\beta = 0, \alpha = \infty$ singularity. The global nature of this singularity is illustrated by the following theorem

Theorem 3.3 (Simon, 1969). *Let $\gamma[0, 1] \to \mathbb{C}$ be a path in the β plane obeying*

1. $\gamma(0) = \gamma(1) \in \mathbb{R}$
2. $\forall t \in [0, 1]$ $(\gamma(t))^* = \gamma(1 - t)$
3. *γ has winding number 3*
4. *$E_n(\alpha, 1)$ is continuable along γ*

Then

$$E_n[\gamma(1), 1] = E_n[\gamma(0), 1], \tag{15}$$

i.e., continuation along a sufficiently nice closed loop γ brings us back to where we started.

Remark. 1. The second conditions essentially requires that γ circles around complex conjugate branch points in complex conjugate ways.

2. This theorem tells us that if we draw branch cuts between complex conjugate points, we get a single-valued function on each sheet.

Proof. $\gamma(\frac{1}{2})$ is real and $E_n(\alpha, 1)$ is real for real α near $\gamma(\frac{1}{2})$. Thus,

$$E_n(\gamma(t), 1) = E_n^*[\gamma(1-t), 1], \tag{16}$$

by the Schwartz reflection principle. Since $E_n[\gamma(0), 1]$ is real, we are done. □

An interesting open question in the field is to prove that $E_n(\alpha, 1)$ can only have isolated singularities (in the finite α plane). Loeffel et al.[6] have shown this is true for $|\arg \alpha| < \frac{2\pi}{3}$. The eigenvalues of $H(\alpha, \beta)$ are the implicit solutions of an equation $\psi(\alpha, E) = 0$, where ψ is an entire function of α and E. It would suffice to show that no function so defined has a natural boundary (and no explicit counter-example appears to be known).[3]

4 Applications of Padé Approximants to the Anharmonic Oscillator

The main result of this section is Loeffel and Martin's proof that any diagonal Padé sequence $[N, N+j]$ formed from the Rayleigh-Schrödinger series for E_n converges to $E_n(1,\beta)$ uniformly on compact subsets of the cut plane.

The convergence of these diagonal Padé approximants leads to interesting possibilities for the Feynman series of a relativistic field theory. For instance, it is conjectured that the convergence of the diagonal Padé approximants is connected to the ground state energy density (=sum of connected vacuum graphs) in a $d = 1+1 \quad \phi^4$ theory.

Theorem 4.1 (Loeffel and Martin, 1969)**.** *The Pade approximants $[N, N+j](x)$ converge as $N \to \infty$ uniformly on compact sets if j is fixed. The limits of these sequences are equal to each other and to $E_n(1,\beta)$.*

Proof. The proof of this theorem is quite involved and uses a series of important results about the analytic properties of the energy levels proved through a series of papers in the 1960s.

The key results used are[3]:

1. $E_n(1,\beta)$, has an analytic continuation to a cut plane, cut along the negative real axis[8]

2. $$\operatorname{Im}\beta = 0 \implies \operatorname{Im} E_n(1,\beta) = 0 \tag{17}$$

3. The Rayleigh-Schrödinger series is asymptotic to $E_(1, \beta)$ as $\beta \to 0$ uniformly in $|\arg \beta| \leqslant \pi$ [3]

4. For β large and fixed n, $|E_n(1, \beta)| \sim C\beta^{\frac{1}{3}}$. This follows from a result of Kato.[9]

Let a_n be the Rayleigh Schrodinger coefficients of $E(1, \beta)$. It is known that

$$a_n = (-1)^{n+1} \int_0^1 \gamma^n \mathrm{d}\rho(\gamma) \tag{18}$$

where

$$\mathrm{d}\rho(\gamma) = \lim_{\epsilon \to 0^+} \frac{1}{\pi\gamma} \operatorname{Im} E(1, -\frac{1}{\gamma} + i\epsilon)\mathrm{d}\gamma \tag{19}$$

$\mathrm{d}\rho(\gamma)$ is a positive measure so $(-a_n)$ defines a Stieltjes series. This casts the proof into what is essentially a moment problem, of inverting the mapping that takes the measure to the sequences of moments. By applying the convergence and analytic properties of Padé approximants we proved in section 2 to Stieltjes series [1], it follows that $[N, N+j]$ converges for any fixed j, say to $f_j(\beta)$. Each f_j obeys the same conditions as $E_n(1, \beta)$, hence both $\mathrm{d}\rho(\gamma)$ and

$$\mathrm{d}\rho_j(\gamma) = \lim_{\epsilon \to 0^+} \frac{1}{\pi\gamma} \operatorname{Im} f_j(-\frac{1}{\gamma} + i\epsilon)\mathrm{d}\gamma \tag{20}$$

solve the moment problem for the (a_n) given in the above equation. Then by a uniqueness theorem of Carleman [1], $\rho = \rho_j$. Thus $f_j - E$ is entire and has a zero asymptotic series. This means that $f_j - E$ is. identically zero i.e.

$f_j = E$. Hence for any fixed j the Padé approximants $[N, N+j]$ converge uniformly to $E_n(1,\beta)$ as $N \to \infty$ $\square$

5 Conclusion

There is, of course, a lot more to say about Padé approximants. Their theory forms a rich body mathematical literature and their applications extend far beyond just the anharmonic oscillator. They appear in analytic number theory through the Riemann-Padé function and in the DLog Pad method. They are also used in the study of differnential equations. They have rich applications in mathematical physics too, including applications to the Ising Model, thermodynamics of lattice gasses, forward scattering amplitude series, the Heisenberg model and the many body problem among others.

The quartic oscillator is simply a gateway to rich mathematics and physics, from the study of polynomial oscillators and multi dimensional oscillators to other systems without analytic solutions. They eventually lead to studies in field theory, and rich and active area of research.

The references provide much greater breadth and depth than can be covered in a single thesis. While I have attempted to select the results most relevant to the single topic I have chosen to study, and present them through a coherent narrative, the interested reader will find the references to be a treasure trove of compelling mathematics on a broad range of topics.

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