PADE APPROXIMANTS AND THE ANHARMONIC OSCILLATOR

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The diagonal Padé approximants of the perturbation series for the eigenvalues of the anharmonic oscillator (a βx^4 perturbation of $p^2 + x^2$) converge to the eigenvalues.

Recently there has been considerable interest in applying the method of Padé approximants [1] to strong interaction physics [2]. This interest is based on the assumption that the diagonal Padé's based on the Feynman series for the partial wave scattering amplitude converge to the "correct answer". We report here a study of the Padé approximants for the energy levels, $E_n(\beta)$, of the anharmonic oscillator whose Hamiltonian is $p^2 + x^2 + \beta x^4$. Our main result is that the diagonal Padé's based on the Rayleigh-Schrödinger series for an x^4 perturbation of $p^2 + x^2$ converge for any eigenvalue and that the limit is the actual eigenvalue.

We feel that this result is of some interest both in itself, and in relation to the work of Bessis et al. and Copley and Masson. The Hamiltonian $p^2 + x^2 + \beta x^4$ is closely analogous to a field theory with the Hamiltonian density $:\pi^2: + :(\nabla\phi)^2: + m^2 :\phi^2: + \beta :\phi^4:$. The analogy is strengthened by the fact that the perturbation series for the Green's function diverge in both cases. For the anharmonic oscillator it has been proved and for the field theory it is hoped that the series is asymptotic to the actual Green's function. What we prove here is that for the *eigenvalues* of the anharmonic oscillator, the Padé approximants formed from the divergent Rayleigh-Schrödinger perturbation series converge to the right answer.

We first recall that the Padé approximants associated with a formal power series, $\sum a_n z^n$, are defined as follows: $f^{[N,M]}$ is that unique rational function of degree M in the numerator and N in the denominator satisfying

$$f^{[N,M]}(z) - \sum_0^{M+N} a_n z^n = O(z^{N+M+1})$$

Our proof of convergence will depend on analytic properties recently established for the anharmonic oscillator energy levels as functions of the coupling constant † [4,5]. Explicitly, we use:

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

We return to a proof of this fact, which is the heart of the argument, near the conclusion of the note.

(b) $\mathrm{Im}\, E_n(\beta)$ 0 if $\mathrm{Im}\, \beta$ 0.

This follows from the simple observation $\mathrm{Im}\, E_n(\beta) = \mathrm{Im}\, \beta\langle x^4\rangle$.

(c) The Rayleigh-Schrödinger series is asymptotic to $E_n(\beta)$ as $\beta \to 0$, uniformly in $|\arg \beta| \leq \pi$.

For β 0, this follows from results of Kato [7]. For arbitrary β, it can be proved directly

† The earliest studies of analyticity used a non-rigorous WKB related approximation [3]. In the field theory case, there are no exact theories whose analytic properties can be similarly analyzed. However, one is very close to a $(\phi^4)_2$ theory for which the Padé approximants might converge [6].

‡ This is a non-trivial statement since $E_n(\beta)$ has infinitely many branch points near β 0 [4]. They happen to be on the second sheet.

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using Hilbert space arguments [4] or from Kato's results and the analytic and positivity properties (a), (b) [5].

(d) For β large and fixed n, $|E_n(\beta)| \quad C|\beta|^{1/3}$ *.

Consider the Hamiltonian $p^2 + \alpha\kappa^2 + \beta\kappa^4$ (α real, $\beta \quad 0$) with eigenvalues $E_n(\alpha, \beta)$. As Symanzik has pointed out [8], since the scaling $p \rightarrow \beta^{1/6} p$; $\kappa \rightarrow \beta^{-1/6}\kappa$ is unitarily implementable, $E_n(1, \beta) = \beta^{1/3} E_n(\beta^{-2/3}, 1)$ for β real. By analytic continuation, this holds in the entire cut β plane. Since $E_n(\alpha, 1)$ is analytic at $\alpha = 0$, the bound follows with any $C \quad E_n(0, 1)$.

(e) Fix n. If a_m are the Rayleigh-Schrödinger coefficients for $E_n(\beta)$, then $a_m \leqslant CD^m m^m$.

This follows from the usual recursive relations for the a_m by an inductive argument [4].

Now one proves that any diagonal Padé sequence, $f^{[N, N+j]}(\beta)$ (j fixed), for an eigenvalue, $E(\beta)$, converges uniformly on compacts of the cut plane. From (a), (b), (c) and (d), it follows that

$$a_n = (-1)^{n+1} \int_0^\infty \gamma^n \mathrm{d}\rho(\gamma) \qquad \text{for} \qquad n \geqslant 1 \tag{1}$$

where

$$\mathrm{d}\rho(\gamma) = \lim_{\epsilon \to 0^+} [\pi\gamma]^{-1} \operatorname{Im} E(-\gamma^{-1} + i\epsilon)\mathrm{d}\gamma \tag{2}$$

From (b), we conclude that $\mathrm{d}\rho(\gamma)$ is a positive measure so that $(-a_n)$ defines a series of Stieltjes. It thus follows from general theorems on Padé approximants [1], that $f^{[N, N+j]}$ converges for any fixed j †, say to $f_j(\beta)$. Each f_j obeys (a), (b), (c) and thus both (2) and

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

solve the moment problem for the (a_n), i.e., obey (1). By (e), $\sum |a_n|^{-1/(2n+1)} = \infty$ so, by a theorem of Carleman [1], $\rho = \rho_j$. Thus $f_j - E$ is entire and has a zero asymptotic series, i.e., $f_j - E = 0$. This completes the proof.

We have made numerical calculations for the ground state to check the rate of convergence of the Padé approximants. In table 1, we list $f^{[20, 20]}(\beta)$ for $\beta = 0.1, 0.2, \ldots, 1.0$ computed using the Rayleigh-Schrödinger coefficients found by Bender and Wu [3]. We compare $f^{[20, 20]}$ with rigorous upper and lower bounds as computed by Bazley-Fox and Reid [9] ‡. We note for comparison that the sum of the first 41 terms of the Rayleigh-Schrödinger series is of order 10^{26}

Table 1
Comparison of Padé with rigorous bounds.

β	Upper bound (a)	Lower bound (b)	$f^{[20, 20]}$ (c)
0.1	1.065 286	1.065 285	1.065 285 509 543
0.2	1.118 293	1.118 292	1.118 292 654 3(57)
0.3	1.164 055	1.164 041	1.164 047 156(234)
0.4	1.204 848	1.204 791	1.204 810 31(0 603)
0.5	1.241 957	1.241 811	1.241 853 9(48 135)
0.6	1.276 195	1.275 909	1.275 983 (105 974)
0.7	1.308 110	1.307 324(·)	1.307 747(246 301)
0.8	1.338 096	1.337 397	1.337 54(1 726 579)
0.9	1.266 442	1.364 349(·)	1.365 66(2 398 911)
1.0	1.393 371	1.392 131	1.392 3(37 481 861)

(a) From Bazley-Fox [12], table 1. A Rayleigh-Ritz method was used on the first five even parity levels.
(b) From Reid [12], table 3 except as noted by (·) which are taken from Bazley-Fox [12].
(c) We have thrown out the last three digits from a double precision answer assuming them insignificant because of round-off error. The figures in parentheses represent digits which are not constant from $f^{[17, 17]}$ on.

Table 2
$f^{[N, N]}(\beta)$ for $\beta \leqslant 1$.

N	β 0.1	β 0.2	β 1.0
1	1.063 829 787 234	1.111 111 111 111	1.272 727 272 727
2	1.065 217 852 490	1.117 540 578 275	1.348 289 096 707
3	1.065 280 680 051	1.118 183 011 861	1.373 799 864 956
4	1.065 285 049 128	1.118 272 722 955	1.383 756 497 228
5	1.065 285 455 329	1.118 288 405 206	1.388 075 603 389
6	1.065 285 502 030	1.118 291 631 128	1.390 103 754 651
7	1.065 285 508 357	1.118 292 382 860	1.391 116 612 108
8	1 065 285 509 335	1.118 292 576 357	1.391 648 018 148
9	1.065 285 509 503	1.118 292 630 404	1.391 938 365 335
10	1.065 285 509 535	1.118 292 646 573	1.392 102 495 074
11	1.065 285 509 541	1.118 292 651 703	1.392 198 009 942
12	1.065 285 509 543	1.118 292 653 416	1.392 255 010 021
13	1.065 285 509 543	1.118 292 654 014	1.392 289 784 380
14	1.065 285 509 543	1.118 292 654 231	1.392 311 424 163
15	1.065 285 509 543	1.118 292 654 313	1.392 325 157 322
16	1.065 285 509 543	1.118 292 654 345	1.392 333 991 014
17	1.065 285 509 543	1.118 292 654 357	1.392 338 973 540
18	1.065 285 509 543	1.118 292 654 358	1.392 339 559 160
19	1.065 285 509 543	1.118 292 654 362	1.392 341 333 864
20	1.065 285 509 543	1.118 292 654 357	1.392 337 481 861

* Using (b) alone, one can prove $|E_n(\beta)| \quad C|\beta|$. This would imply (1) for $n \quad 2$ which would suffice for our results.

† In ref. 1, this is only proved for $j \quad 0$, when eq. (1) holds! However, $(-E(\beta))^{-1}$ obeys (a)-(d) with the inverse power series so $(-E^{-1})^{[N, N+j]} \quad -E^{[N+j, N]}$ converges. One of us (B.S.) would like to thank Professor D. Masson for a discussion of this point.

‡ Notice that we give this lower bound only as a check of the numerical calculations. Indeed $f^{[N, N]}$, for positive β is itself necessarily a lower bound of $E(\beta)$.

even for $\beta = 0.1$. In table 2, we show the rate of convergence of $f^{[N,N]}(\beta)$. This get worse as β increases which is to be expected since $f^{[N,N]}(\beta) \sim$ some constant C_N as $\beta \to \infty$ while $E(\beta) \sim C\beta^{1/3}$ as $\beta \to \infty$.

Let us return to the proof of (a), the cut plane analyticity for $E_n(\beta)$. The absence of poles and non ramified isolated essential singularities for Im $\beta \neq 0$ is a direct consequence of the Herglotz property (b) [4,5]. When β is real and positive, analyticity is a consequence of the Kato-Rellich theorems on regular perturbations.

To eliminate natural boundaries and branch points a more detailed study is needed [5]. The best characterization of an energy level for real α and β 0 is the number of zeros of its wave function in x space. It turns out that this notion can be generalized to complex α and β. Let us start from the wave equation

$$H\psi = \left(-\frac{d^2}{dx^2} + \alpha x^2 + x^4\right)\psi = E(\alpha, 1)\psi(x, \alpha, E)$$

with the boundary condition

$$\psi \sim \frac{1}{x} \exp - \tfrac{1}{3}x^3 \qquad \text{for} \qquad x \to +\infty$$

The energy levels are given implicitly by

$$\psi(x = 0, \alpha, E) = 0 \qquad \text{for odd levels}$$

$$\frac{\partial}{\partial x}\psi(x = 0, \alpha, E) = 0 \qquad \text{for even levels}$$

where $\psi(x = 0, \alpha, E)$ is entire in α and E. Around a point $\alpha_0 E_0$, where E_0 is finite, the energy is an analytic function of a fractional power of $\alpha - \alpha_0$.

What we can prove by integrating $\psi^*(z)[H - E] \times \times \psi(z)$ along rays in the complex z plane is the following: for $|\arg\alpha|$ $\frac{2}{3}\pi - \epsilon$, ϵ arbitrarily small, $|\psi|$ is strictly positive for

$$\tfrac{1}{6}\pi - \epsilon' \quad \arg z \quad \tfrac{1}{6}\pi \quad \text{and} \quad -\tfrac{1}{6}\pi < \arg z < -\tfrac{1}{6}\pi + \epsilon'$$

and for $|z|$ large if $|\arg z|$ $\frac{1}{6}\pi$. Therefore if we vary α continuously and hence E continuously (*if it does not go through infinity*) the number of zeros of the wave functions in the sector $|\arg z| <$ $< \frac{1}{6}\pi$ cannot vary. That E will remain bounded during this continuous motion in the α plane is established as follows: when we start, with α on the real axis, we have a finite number of zeros n in this sector, all of which are real. Now integrating the wave equation from the origin in the Volterra form we can prove that $E|$ cannot get too large for complex α because if it did the "free" solution $\sin(\sqrt{E}z)$ or $\cos(\sqrt{E}z)$ would dominate for finite $|z|$ and, applying the Rouché theorem to a suitable finite region inside $|\arg z|$ $\frac{1}{6}\pi$ we would get a number of zeros larger than n, which would be a contradiction *.

Since E remains bounded, the only possible singularities of $E(\alpha)$ are branch points. However, if we turn around such a branch point and come back to the real axis we fall back on a real wave function with the *same* number of zeros z as the one we started from. Therefore there cannot be any branch point for $|\arg\alpha|$ $\frac{2}{3}\pi$. If we return through scaling to the variable β we find that all energy levels $E_n(\beta)$ are analytic in a cut plane.

Finally let us discuss the extension to κ^{2m} perturbations and several dimensions. For κ^{2m} perturbations, there are indications that $a_n \sim \sim CD^n n^{(m-1)n}$ so that Carleman's criterion $\sum |a_n|^{-1/(2n+1)} = \infty$ breaks down at κ^8. Since Carleman's criterions is sufficient but not necessary, our proof that $f_j = E$ breaks down but the equality may still hold. A numerical analysis of this κ^8 problem is in progress [10]. Similarly for several dimensional coupled anharmonic oscillators, one part of the proof breaks down: for the proof that $E_n(\beta)$ has no branch points in the cut plane depends on keeping track of zeros, a more complicated affair in several variables.

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* We hope to find an argument which does not make explicit use of the wave equation to show that E remains bounded, but the matter is not yet completely clear. It would obviously be better for it could be generalized to more degrees of freedom.

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