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Accurate summation of the perturbation series for periodic eigenvalue problems

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Abstract. We show that algebraic approximants prove suitable for the summation of the perturbation series for the eigenvalues of periodic problems. Appropriate algebraic approximants constructed from the perturbation series for a given eigenvalue provide information about other eigenvalues connected with the chosen one by branch points in the complex plane. Such approximants also give those branch points with remarkable accuracy. We choose Mathieu's equation as illustrative example.

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1 Introduction

Perturbation theory is one of the most widely used approximate methods in quantum mechanics. It was applied to most fundamental problems at the very dawn of wave theory. In addition to its intrinsic simplicity, a strong appeal of perturbation theory is that it provides useful analytical expressions for the properties of a number of physically motivating models. For that reason such an approach is commonly discussed in most textbooks on quantum mechanics and quantum chemistry.

In order to perform accurate numerical perturbation calculations it is necessary to obtain sufficient perturbation coefficients, and to sum the series. It likely happens that the perturbation expansion is either divergent or slowly convergent; for that reason many general and particular approaches are currently available to overcome such problems [1]. Recently, there has been great interest in algebraic approximants that are implicit polynomial approximations to multiple-valued functions constructed from their Taylor series [2–4]. The well-known Padé approximants [5] are the linear version of algebraic approximants; those of higher degree prove more suitable for the treatment of complex functions with real perturbation series. For example, such algebraic approximants enable an adequate description of multiple-valued functions, resonance energies, and branch points [2–4].

The radius of convergence of a perturbation series is typically limited by square-root branch points, where two eigenvalues merge at complex values of the perturbation parameter which is commonly real in the physical application. Because such eigenvalues are therefore branches of a multiple-valued function, one expects that an adequate approximation based on the perturbation series for one of the eigenvalues gives results for both of them. Such a possibility has not been taken into account in current practical applications of perturbation theory, except for some recent treatment of anharmonic oscillators [3].

The purpose of this paper is to show that algebraic approximants properly constructed from the perturbation series for a given eigenvalue provide results also for other eigenvalues that merge with it. In order to illustrate this striking feature of the algebraic approximants we choose Mathieu's equation because it has been widely studied, its main properties are well-known, and there are many results available for comparison [6–10]. We believe that Mathieu's equation provides a more dramatic example than the anharmonic oscillators; notice that both models differ substantially because the characteristic values of the former have finite radii of convergence.

In Section 2 we briefly review the construction of a particular class of algebraic approximants, in Section 3 we outline those properties of Mathieu's equation that are relevant for the present paper and show results of the application of algebraic approximants to the perturbation series for some characteristic values.

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2 Algebraic approximants

Perturbation theory provides an approximation to a physical quantity E in the form of a power series of a perturbation parameter λ:

$$E = \sum_{j=0}^{\infty} E_j \lambda^j. \tag{1}$$

Sometimes this perturbation expansion is either divergent, slowly convergent, or its radius of convergence is too small for the physical application. In such a case one resorts to one of the many methods that improve the convergence properties of power series. Here we are concerned with algebraic approximants that are implicit expressions of the form [3]

$$\sum_{n=0}^{N} p_n(\lambda) E^n = 0, \; p_n(\lambda) = \sum_{m=0}^{M_n} p_{nm} \lambda^m. \tag{2}$$

We choose the independent adjustable parameters p_{nm} in such a way that one of the roots of equation (2) satisfies

$$E = \sum_{j=0}^{P} E_j \lambda^j + \mathcal{O}(\lambda^{P+1}), \; P = N + \sum_{n=0}^{N} M_n - 1. \tag{3}$$

This condition completely determines the value of all those coefficients.

The root of equation (2) that satisfies (3) provides an approximation to $E(\lambda)$ that is much more accurate than the partial sum (3). As P increases the estimate given by the algebraic approximant may converge to the actual value of $E(\lambda)$ even when the radius of convergence of the original perturbation series (1) is zero [2–4].

Padé approximants, by far the most popular algebraic approximants, are the linear version of equation (2), which follows when $N = 1$ [5]. These approximants are not suitable for the description of a function $E(\lambda)$, with real Taylor coefficients E_j, that yields complex values for real λ. In such a case algebraic approximants of higher degree ($N > 1$) may give the right answer [2–4].

When $N > 1$ the approximate value of $E(\lambda)$ is given by the root that satisfies (3); the remaining roots may be spurious or may represent meaningful branches of the function $E(\lambda)$ [2,3].

One can construct many algebraic approximants of the form (2) from the same partial sum (3). In some cases trial and error is the only way to determine a convergent sequence [3], in others it is possible to profit from information about the function $E(\lambda)$ in order to restrict the enormous flexibility of the algebraic approximants. For example, suppose that the unknown function $E(\lambda)$ satisfies another expansion of the form

$$E(\lambda) = \lambda^{\alpha} \sum_{j=0}^{\infty} e_j \lambda^{-\beta j}, \; \alpha, \, \beta > 0. \tag{4}$$

In such a case one may force the roots of the algebraic approximants to obey equation (4) even when one does not know the actual value of the coefficients e_j.

Extensive and judicious numerical investigation of the application of algebraic approximants to the Rayleigh-Schrödinger perturbation series for anharmonic oscillators showed that only those algebraic approximants with roots that behave asymptotically as $e_0\lambda^{\alpha}$ converged towards the actual eigenvalues [3]. Such results have led to think that the best algebraic approximants are those that exhibit roots that behave asymptotically as shown by equation (4). Such particular algebraic approximants, which have been named *intelligent*, have proved to give accurate results for anharmonic oscillators [4], and simpler versions of them were applied to the Zeeman effect in hydrogen some time ago [11].

The intelligent approximants studied so far are of the form

$$\sum_{m=0}^{M} \sum_{j=0}^{J_m} C_{mj} \lambda^m E^{N-(m+j\beta)/\alpha} = 0, \; J_m = [(\alpha N - m)/\beta], \tag{5}$$

where $[x]$ denotes the greatest integer smaller than or equal to x. The condition that a Taylor expansion of a root of this approximant gives the partial sum (3) of order

$$P = M - 1 + \sum_{m=0}^{M} J_m, \tag{6}$$

completely determines the coefficients C_{mj} as solutions of a system of linear equations. We do not show it here because its derivation is straightforward; suffice to say that it gives the $C_{mj}{}'s$ in terms of the $E_j{}'s$.

Substituting $\lambda^{\alpha} W$ for E into equation (5) and dividing the resulting expression by $\lambda^{\alpha N}$ we obtain

$$\sum_{m=0}^{M} \sum_{j=0}^{J_m} C_{mj} \lambda^{-j\beta} W^{N-(m+j\beta)/\alpha} = 0, \tag{7}$$

which shows that the roots of the approximant (5) can also be expanded as

$$E = \lambda^{\alpha} \sum_{j=0}^{\infty} W_j \lambda^{-j\beta}. \tag{8}$$

If the coefficients W_j approach the coefficients e_j of the expansion (4) as P (and thereby M and N) increases, then we expect the intelligent approximants to give $E(\lambda)$ accurately for all values of λ.

3 Mathieu's equation

For the present investigation we choose Mathieu's equation because there is much information about its solutions [6–10]. Mathieu's equation exhibits many physical applications in various fields and is commonly written in several different ways; here we adopt one of the most popular forms [7]:

$$Y''(x) + [a - 2q\cos(2x)]Y(x) = 0. \tag{9}$$

Table 1. Characteristic values $a_{2m}(q = 0) = 4m^2$ from intelligent approximants $IA[M, 2M]$ constructed by means of the perturbation series for a_0.

M	a_0	a_2	a_4	a_6	a_8	a_{10}	a_{12}
1	0	4.571428571					
2	0	3.999988900	17.22312897	40.41373362			
3	0	4.000000000	15.99860111	38.30568114	69.27730642	113.5096445	
4	0	4.000000000	15.99999983	36.03235035	60.28735302	109.7781708	
5	0	4.000000000	16.00000000	36.00001544	64.24016225	91.35774738	146.6106583
6	0	4.000000000	16.00000000	36.00000000	64.00001914	100.1287412	139.7666807
7	0	4.000000000	16.00000000	36.00000000	63.99999991	100.0008080	143.7082723
8	0	4.000000000	16.00000000	36.00000000	64.00000000	100.0000009	143.9827301
9	0	4.000000000	16.00000000	36.00000000	64.00000000	100.0000000	143.9999978

There are four types of periodic solutions that admit Fourier expansions of the form [7]

$$Y(x) = \sum_{m=0}^{\infty} A_{2m+p} \cos[(2m+p)x], \quad a = a_{2m+p},\ p = 0, 1, \tag{10}$$

$$Y(x) = \sum_{m=0}^{\infty} B_{2m+p} \sin[(2m+p)x], \quad a = b_{2m+p},\ p = 0, 1. \tag{11}$$

It is not our purpose to summarize all the properties of Mathieu's equation and its characteristic values $a(q)$ that one encounters elsewhere [6,7]. Suffice to say that straightforward perturbation theory yields approximate solutions in the form of power series:

$$Y(q, x) = \sum_{j=0}^{\infty} Y_j(x) q^j,\ a(q) = \sum_{j=0}^{\infty} c_j q^j, \tag{12}$$

and that the calculation of as many exact perturbation coefficients $Y_j(x)$ and c_j as desired offers no difficulty. This is another reason for choosing Mathieu's equation in the present investigation. One finds the first coefficients of the perturbation series (12) for the four types of periodic solutions (10, 11) in current literature [6,7].

In addition to the q-power series the characteristic values can also be expanded as [6,10]

$$a(q) = q \sum_{j=0}^{\infty} w_j q^{-j/2} = q[-2 + 2(2n+1)q^{-1/2} - \frac{1}{4}(2n^2 + 2n + 1)q^{-1} + \ldots],\ n = 0, 1, \ldots \tag{13}$$

Consequently, we can build intelligent approximants as indicated in the preceding section for $E = a$. Because $a_{2m}(-q) = a_{2m}(q)$ and $b_{2m}(-q) = b_{2m}(q)$ the perturbation coefficients of odd order for these characteristic values vanish [6,7]. Choosing the perturbation parameter to be $\lambda = q^2$ we realize that $\alpha = 1/2$ and $\beta = 1/4$. In order to avoid the fractional powers of E that will otherwise appear in the algebraic approximants (5) we set $C_{m\,2j+1} = 0$. As we will shortly see, the fact that the variable of the asymptotic expansion of the roots of the intelligent approximants results to be q^{-1} instead of $q^{-1/2}$ does not affect the results unfavorably, and we gain some simplicity in the calculation. The remaining characteristic values satisfy $a_{2m+1}(-q) = b_{2m+1}(q)$ and $\lambda = q$ is a suitable perturbation parameter for them. In this case $\alpha = 1$ and $\beta = 1/2$, and again we avoid the occurrence of fractional powers of E exactly as discussed above.

The perturbation series for the characteristic values of Mathieu's equation have finite radii of convergence determined by square-root branch points at which a pair of characteristic values cross in the complex q plane. For example, it has been found that $a_{2m+p} = a_{2m+p+2}$, where $m = 0, 1, \ldots$, and $b_{2m+p} = b_{2m+p+2}$, where $m = 1, 2, \ldots$, at those branch points. Accordingly, we can view the characteristic values as branches of a multiple-valued function $a(q) = E(\lambda)$, and expect that the intelligent approximants constructed from the perturbation series for a given characteristic value (for example a_{2m}) give results for other characteristic values corresponding to solutions of the same symmetry and period. From now on $IA[M, N]$ will denote an intelligent approximant of degrees M and N. In particular we concentrate on the case $N = 2M$ which requires a perturbation series of order $P = (M + 1)^2 - 2$ when $\alpha = 1/2$ and $\beta = 1/4$.

We first consider intelligent approximants constructed from the perturbation series for the characteristic value a_0. Table 1 shows roots of the approximants $IA[M, 2M]$ for $q = 0$ that converge towards $a_{2m}(q = 0) = 4m^2$, $m = 0, 1, \ldots$ as M increases. Obviously, by construction the case $m = 0$ is exact for all values of M. Table 2 compares roots of the intelligent approximant $IA[7, 14]$ with the first characteristic values a_{2m} obtained by means of a reliable nonperturbative calculation. The latter consists of solving $A_{2k}(a, q) = 0$ for increasing values of k till all the selected roots become stable to a given accuracy. We have purposely chosen q-values that appear in current literature [7] in order to verify present perturbative and nonperturbative results.

We clearly see that the roots of the intelligent approximants converge, not only to the characteristic value chosen to construct them (a_0 in the cases above), but also to all

Table 2. Characteristic values $a_{2m}(q)$ from the intelligent approximant $IA[7,14]$ constructed by means of the perturbation series for a_0. The second value for each entry comes from a nonperturbative method.

q	a_0	a_2	a_4	a_6	a_8	a_{10}
5	−5.800046021	7.449109740	17.09658168	36.36089998	64.19884	100.127
	−5.800046021	7.449109740	17.09658168	36.36089998	64.19884239	100.1263692
10	−13.93697996	7.717369850	21.10463371	37.53360634	64.80089	100.508
	−13.93697996	7.717369850	21.10463371	37.53360634	64.80089101	100.5067700
15	−22.51303776	5.077983198	25.37506106	39.96816628	65.82799	101.146
	−22.51303776	5.077983198	25.37506106	39.96816628	65.82799493	101.1452034
20	−31.31339007	1.154282885	27.59457815	44.06294865	67.34588	102.050
	−31.31339007	1.154282885	27.59457815	44.06294865	67.34587524	102.0489160
25	−40.25677955	−3.522164727	27.80524058	48.97578672	69.52407	103.231
	−40.25677955	−3.522164727	27.80524058	48.97578672	69.52406517	103.2302048

the other characteristic values (corresponding to the same parity and period) of which the approximants have received no information whatsoever. The conclusion is that the intelligent approximants already approach a multiple-valued function whose branches are the characteristic values of Mathieu's equation. As expected the accuracy of the estimated a_{2m} decreases as m increases.

In order to verify if intelligent approximants are really the most accurate algebraic approximants that one can build for a given problem, we have constructed diagonal staircase sequences of algebraic approximants labelled by two subscripts, m (the order of the polynomial function of E) and n (determined by the order of the perturbation series used in the construction) [3]. For a given value of n the accuracy of the algebraic approximants increases, reaches a maximum, and then decreases as m increases. Figure 1 shows the logarithmic error of the diagonal staircases of algebraic approximants for $a_2(0)$ (continuous lines), constructed from the perturbation series for a_0, as functions of m, and for some such values of n for which we can also build intelligent approximant $IA[M,2M]$ (broken lines in that figure). Notice that the accuracy of a given intelligent approximant is always comparable to the greatest accuracy of the corresponding diagonal staircase. We draw similar conclusions for other characteristic values, and for other values of q.

It also follows from the results in Table 2 that the algebraic approximants continue a perturbation series beyond its radius of convergence. For example, the perturbation series for a_0 is known to diverge for all $|q| > 1.468\,768\,613\,785\,14$ (see below), and Table 2 shows that the approximants converge for much greater values of $|q|$.

We have repeated the calculations choosing the perturbation series for a_{10}. Results in Table 3 show that the accuracy of the approximate a_{2m} decreases as $|m-10|$ increases and that this effect is less noticeable for smaller than for larger values of m.

The intelligent approximants give us implicit equations of the form $IA(E,\lambda) = 0$ from which we obtain either $E(\lambda)$ or $\lambda(E)$. It is well-known that $\mathrm{d}\lambda/\mathrm{d}E = 0$ and $\mathrm{d}^2\lambda/\mathrm{d}E^2 \neq 0$ at a square-root branch point of $E(\lambda)$ [12].

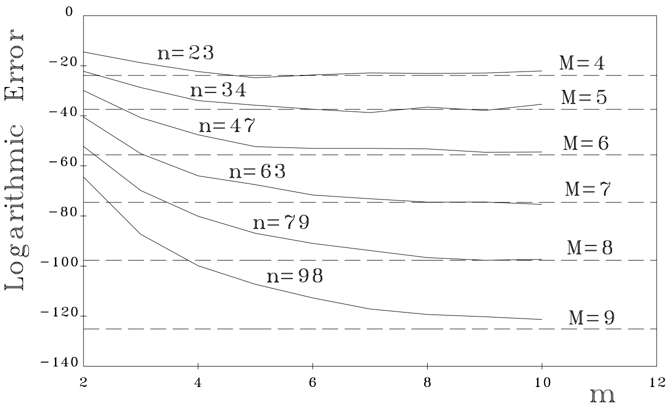

Fig. 1. Logarithmic error in the calculation of $a_2(0)$ by means of diagonal staircases of algebraic approximants (continuous lines) and intelligent approximants (broken lines) constructed from the perturbation series for a_0.

Consequently, if the approximants are sufficiently accurate in a neighborhood of a branch point we should be able to obtain its parameters from the system of nonlinear equations [12]

$$IA(E,\lambda) = 0, \ \frac{\partial IA(E,\lambda)}{\partial E} = 0. \tag{14}$$

Moreover, if the intelligent approximants provide a sufficiently accurate representation of the multiple-valued function $E(\lambda) = a(q)$, then one expects that the approximants constructed from a_{2m} will give not only the branch points (a_{2m-2}, a_{2m}) and (a_{2m}, a_{2m+2}) but also other branch points (a_{2k}, a_{2k+2}) in the complex q-plane. As an example, Table 4 shows the rate of convergence of the solutions of equation (14) (with intelligent approximants constructed from the perturbation series for a_0) towards one of the branch points (a_4, a_6). Table 5 shows other branch points obtained by means of the intelligent approximant $IA[7,14]$ built from the same perturbation series. Comparison with precise nonperturbative calculations [9,10] shows that the accuracy of the branch points (a_{2m}, a_{2m+2}) thus obtained decreases as m increases.

Table 3. Characteristic values $a_{2m}(q)$ from the intelligent approximant $IA[7, 14]$ constructed by means of the perturbation series for a_{10}. The second value for each entry comes from a nonperturbative calculation.

q	a_0	a_2	a_4	a_6	a_8	a_{10}
0	−0.05	4.005	15.9994	36.000009	64.00000000	100.0000000
	0	4	16	36	64	100
5	−5.802	7.4506	17.0961	36.360908	64.19884239	100.1263692
	−5.800046021	7.449109740	17.09658168	36.36089998	64.19884239	100.1263692
10	−13.938	7.7180	21.1045	37.533613	64.80089101	100.5067700
	−13.93697996	7.717369850	21.10463371	37.53360634	64.80089101	100.5067700
15	−22.5139	5.0783	25.37500	39.968170	65.82799493	101.1452034
	−22.51303776	5.077983198	25.37506106	39.96816628	65.82799493	101.1452034
20	−31.3140	1.1546	27.59455	44.062950	67.34587524	102.0489160
	−31.31339007	1.154282885	27.59457815	44.06294865	67.34587524	102.0489160
25	−40.258	−3.5219	27.80523	48.9757870	69.52406517	103.2302048
	−40.25677955	−3.522164727	27.80524058	48.97578672	69.52406517	103.2302048

q	a_{12}	a_{14}	a_{16}
0	144.0000002	195.95	245.0
	144	196	256
5	144.0874476	196.02	250.0
	144.0874473	196.0641161	256.0490256
10	144.3502082	196.21	250.0
	144.3502080	196.2566275	256.1961748
15	144.7895541	196.53	250.0
	144.7895539	196.5780262	256.4416654
20	145.4076591	196.98	250.0
	145.4076589	197.0291433	256.7858628
25	146.2076908	197.56	251.0
	146.2076906	197.6111649	257.2292849

Table 4. Convergence of the roots of equation (14) towards the branch point (a_4, a_6).

M	a	q^2
3	28.7367023964213	−288.912493849802
4	27.3522602213187	−271.604891332361
5	27.3191265168391	−271.299291842535
6	27.3191276740201	−271.299305850403
7	27.3191276740344	−271.299305850470
Ref. [9]	27.31912767	−271.2993058

All the perturbative and nonperturbative calculations described here have been carried out by means of Maple [13]. For example, we obtained the coefficients of the perturbation series for the characteristic values and the intelligent approximants in exact analytical form, and then calculated the roots numerically by means of the command *fsolve*. In order to solve the system of nonlinear equations (14) we resorted to the Newton-Raphson algorithm. Setting the precision of the floating-point arithmetic sufficiently large, one diminishes the unwanted accumulation of round-off errors.

4 Further comments and conclusions

It is not our purpose to put forward the best method for the solution of periodic eigenvalue problems. Perturbation theory is not the fastest or most accurate approach for such a calculation, even with the aid of algebraic approximants. In fact the simple nonperturbative method mentioned above is preferable for all those calculations. The aim of this paper is to call attention on the curious and not so well documented fact that under certain conditions algebraic approximants enable one to obtain several eigenvalues from the perturbation series for one of them. More precisely, present results strongly suggest that algebraic approximants, and in particular intelligent approximants, provide adequate description of the multiple-valued functions whose branches are the eigenvalues of periodic differential equations. This feature, also encountered in other eigenvalue problems [3], may be useful, for example, when the perturbation series is the only approach to a physical quantity.

We have drawn similar conclusions from a well-known perturbed rigid rotor [14], but we do not show those unpublished results here because they do not add anything new to the present discussion. We believe that the

Table 5. Branch points (a_{2m}, a_{2m+2}) from the approximant $IA[7,14]$ constructed by means of the perturbation series for a_0. The second value for each entry comes from reference [9].

m	$\Re a$	$\Im a$	$\Re q^2$	$\Im q^2$
0	2.08869890274970	0	−2.15728124084033	0
	2.08869890	0	−2.15728123	0
2	12.7997162446345	2.76304491692944	0.719587820073328	52.8210579760997
	12.79971624	2.76304492	0.7195878054	52.82105792
4	27.31912767403	0	−271.29930585047	0
	27.31912767	0	−271.2993058	0
4	33.5401564323667	6.362518783972	157.14271175421	279.545558315172
	33.54015643	6.36251878	157.1427118	279.5455584
6	52.0253450	5.55189445	−680.0891251	628.197253
	52.02534500	5.55189444	−680.0891251	628.1972535
6	64.21313050	10.43474553	771.1220885	809.8534122
	64.21313050	10.43474552	771.1220883	809.8534127
8	80.660	0	−2285.45	0
	80.65826424	0	−2285.410357	0
8	86.7946	12.6983	−899.01	2243.272
	86.79479850	12.69861754	−899.0235017	2243.276892
8	104.7906	14.8376	2294.777	1778.871
	104.79053631	14.83777144	2294.771957	1778.873182
10	118.8	8.4	−4289.0	2270.0
	119.40038738	8.20296334	−4318.046781	2295.130833

argument above for Mathieu's equation is sufficiently clear to make our point.

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