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Summation of asymptotic expansions of multiple-valued functions using algebraic approximants: Application to anharmonic oscillators

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Abstract. The divergent Rayleigh–Schrödinger perturbation expansions for energy eigenvalues of cubic, quartic, sextic and octic oscillators are summed using algebraic approximants. These approximants are generalized Padé approximants that are obtained from an algebraic equation of arbitrary degree. Numerical results indicate that given enough terms in the asymptotic expansion the rate of convergence of the diagonal staircase approximant sequence increases with the degree. Different branches of the approximants converge to different branches of the function. The success of the high-degree approximants is attributed to their ability to model the function on multiple sheets of the Riemann surface and to reproduce the correct singularity structure in the limit of large perturbation parameter. An efficient recursive algorithm for computing the diagonal approximant sequence is presented.

1. Introduction

The Schrödinger equation $H\psi = E\psi$, where

$$H = \tfrac{1}{2}p^2 + \tfrac{1}{2}x^2 + \lambda x^\beta \tag{1}$$

gives rise to a well known example of singular perturbation theory (Bender and Orszag 1978). This problem is of physical interest, as a prototypical quantum field theory and as a model for molecular vibrations, and of mathematical interest, on account of the rich singularity structure of the function $E(\lambda)$. A characteristic feature of $E(\lambda)$ is an infinite sequence of branch points approaching a limit point at $\lambda = 0$. (Bender and Wu 1969, Simon 1970, Shanley 1986, Alvarez 1995, Bender and Orszag 1978 pp 350–61). The asymptotic expansions for the energy, $E(\lambda) \sim \sum_{n=0}^{\infty} E_n \lambda^n$, are therefore divergent for all $\lambda \neq 0$. These expansions have become a standard test case for new summation procedures (Reid 1967, Graffi *et al* 1970, Seznec and Zinn-Justin 1979, Caswell 1979, Dmitrieva and Plindov 1980, Drummond 1981, Čížek and Vrscay 1982, Cohen and Kais 1986, Weniger *et al* 1993), in part because the E_n can be easily computed even for extremely large n.

The multiple-valued nature of $E(\lambda)$ causes trouble for summation approximants that are single valued. Consider for example the quartic oscillator, $\beta = 4$. It can be proved in that case (Loeffel *et al* 1969) that $E(\lambda)$ is Padé summable as long as $|\arg\lambda| < \pi$. In practice, the approximants place a sequence of poles along the negative real axis, simulating a branch cut (Baker 1975). The convergence slows as $|\arg\lambda|$ approaches π and fails completely at π. If λ is pure real and negative then the eigenvalue corresponds to a double-valued complex

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resonance energy, $E = E_r \pm i\Gamma/2$, where Γ can be identified, at least approximately, with the resonance width (Connor and Smith 1981). The plus and minus signs correspond to the incoming and outgoing wave boundary conditions respectively. Since the E_n are real the Padé approximants for negative real λ are also real, and cannot converge to the correct result.

The Padé approximant $E_{[L,M]}(\lambda)$ is a rational function $P_L(\lambda)/Q_M(\lambda)$ with a Taylor expansion that reproduces the expansion of $E(\lambda)$ up to given order. P_L and Q_M are polynomials of degree L and M respectively that satisfy the linear equation

$$P(\lambda) - Q(\lambda)E(\lambda) = O(\lambda^{L+M+1}). \tag{2}$$

'$E(\lambda)$' in (2) represents the power series in λ. A natural generalization for double-valued functions is a quadratic Padé approximant (Shafer 1974). The $[L, M, N]$ quadratic approximant is a function of three polynomials A, B and C, of degree L, M and N, respectively, that satisfy

$$A(\lambda) + B(\lambda)E(\lambda) + C(\lambda)E^2(\lambda) = O(\lambda^{L+M+N+2}). \tag{3}$$

The approximant $E_{[L,M,N]}(\lambda)$ is given by the quadratic equation

$$A(\lambda) + B(\lambda)E_{[L,M,N]}(\lambda) + C(\lambda)E^2_{[L,M,N]}(\lambda) = 0 \tag{4}$$

with the double-valued solution

$$E_{[L,M,N]}(\lambda) = \frac{1}{2}\left\{-\frac{B(\lambda)}{A(\lambda)} \pm \left[\frac{B^2(\lambda)}{A^2(\lambda)} - 4\frac{C(\lambda)}{A(\lambda)}\right]^{1/2}\right\}. \tag{5}$$

Convergence theorems for these approximants exist for certain special cases (Baker and Graves-Morris 1996 pp 544–69), but in practice applicability to functions of physical interest has been justified numerically (Short 1979, Jeziorski *et al* 1980, Liu and Bergersen 1981, Common 1982, Mayer and Tong 1985, Vaĭnberg *et al* 1986, De'Bell 1992, Goodson *et al* 1992, Hamer *et al* 1992, Germann and Kais 1993). These approximants do not need to simulate the branch cut with poles; they explicitly contain square-root branch points. For the quartic oscillator they converge at negative real λ (Sergeev 1995).

In the same spirit, an algebraic approximant of arbitrary degree m (Short 1979, Brak and Guttmann 1990) can be defined by the equation

$$\sum_{k=0}^{m} A^{(k)}(\lambda)E^k_{[p_0,p_1,\ldots,p_k]}(\lambda) = 0 \tag{6}$$

where $A^{(k)}(\lambda)$ are polynomials in λ of degree p_k that satisfy

$$\sum_{k=0}^{m} A^{(k)}(\lambda)E^k(\lambda) = O(\lambda^{n+1}) \qquad n = m - 1 + \sum_{k=0}^{m} p_k. \tag{7}$$

This is a special case of a class of summation schemes known collectively as Padé-Hermite approximation (Hermite 1893, Padé 1894, Della Dora and Di Crescenzo 1979, Baker and Graves-Morris 1996 pp 524–69). We will use high-degree algebraic approximants to sum the expansion of the multiple-valued oscillator eigenvalue.

The paper of Short (1979) is the closest prototype of this study. Similar multiple-valued approximants were constructed so as to incorporate the known branch-point structure of Feynman matrix elements. For the multiple-valued function $\ln(1 - z)$, Short observed that quadratic approximants reduce the error by roughly two orders of magnitude compared with Padé approximants. He found similar improvement in accuracy for quadratic and especially cubic approximants for certain Feynman integrals and found that these approximants provide,

in effect, analytic continuations of the asymptotic expansion from the first Riemann sheet to the second.

Here we present a further demonstration of the power of algebraic approximants to describe functions with complicated branch-point structure. We find that the convergence for the ground-state energy of anharmonic oscillators improves with approximant degree, given enough terms in the expansion. High-degree approximants yield very high accuracy for the principal value of $E(\lambda)$ and reasonably good results on higher sheets. Certain choices of the approximant indices give the known large-λ singularity structure, and the corresponding numerical results are especially accurate. Section 2 presents an efficient algorithm for computing algebraic approximants. Section 3 analyses the singularity structure of the approximants and in section 4, as a simple demonstration, we determine the rate of convergence for the infinite-valued function $\lambda^{-1}\ln(1+\lambda)$. Section 5 contains results for quartic, cubic, sextic and octic oscillators.

2. Computational algorithm

The most direct method for calculating algebraic approximants is to solve the system of $n+1$ linear homogeneous equations for the coefficients of the polynomials $A^{(0)}, A^{(1)}, \ldots, A^{(m)}$, that follows from (7) after collecting terms by powers of λ (Della Dora and Di Crescenzo 1979). This approach is appropriate for low-order analyses, but the number of arithmetic operations increases very rapidly with increasing n.

For the conventional 'linear' Padé approximants ($m = 1$) the $[L, M]$ approximants with $L \approx M$ tend in general to be the most accurate (Baker 1975). Our experience is that quadratic and higher-degree approximants with approximately equal indexes are also the most accurate. Here we present an algorithm for computing such approximants that is much faster and needs much less computer memory at large orders than solving the system of linear equations. It yields what we will call the *diagonal staircase* sequence of degree-m approximants, $E_{\{m,n\}}(\lambda)$, $n = m-1, m, m+1, m+2, \ldots$, with

$$\{m,n\} \equiv \left[\underbrace{j, j, \ldots, j}_{i}\,\underbrace{j-1, j-1, \ldots, j-1}_{m+1-i}\right] \tag{8}$$

where j satisfies the equation $(m+1)j = n - i + 2$ with $1 \leqslant i \leqslant m+1$. Table 1 lists representative examples of the index sequences, illustrating the correspondence between $\{m,n\}$ and $[p_0, \ldots, p_m]$.

Our algorithm is an extension to arbitrary degree of the Berlekamp–Massey algorithm (Baker and Graves-Morris pp 153–66). It was used previously by Mayer and Tong (1985) for calculating quadratic approximants and is a special case of a more general algorithm, for Padé–Hermite approximants, derived by Sergeev (1986). Let $R_n(\lambda)$ be a sequence of residual functions such that

$$\sum_{k=0}^{m} A_n^{(k)} E^k(\lambda) = \lambda^{n+1} R_n(\lambda). \tag{9}$$

Note that we have added the subscript n to $A^{(k)}$, to indicate which $E_{\{m,n\}}$ it corresponds to in the diagonal staircase sequence. We will assume that $r_{n,0} \neq 0$ for all n.

The lowest-order approximant of degree m will have each $A_n^{(k)}(\lambda)$ equal to a constant. Any solution for the set $\{A_n^{(0)}, A_n^{(1)}, \ldots, A_n^{(m)}\}$ can be multiplied by a common non-zero factor. Thus, one of these constants is arbitrary. The remaining m constants are determined from the accuracy-through-order conditions, (7). The lowest-order approximant corresponds

Table 1. Indices of approximants that comprise the diagonal staircase sequences. m is the degree of the approximant and n is the highest order in the asymptotic expansion that is needed in the calculation. The entries $[p_0, p_1, \ldots, p_m]$ give the degrees of the constituent polynomials.

n	$m=1$	$m=2$	$m=3$	$m=4$
0	[0, 0]			
1	[1, 0]	[0, 0, 0]		
2	[1, 1]	[1, 0, 0]	[0, 0, 0, 0]	
3	[2, 1]	[1, 1, 0]	[1, 0, 0, 0]	[0, 0, 0, 0, 0]
4	[2, 2]	[1, 1, 1]	[1, 1, 0, 0]	[1, 0, 0, 0, 0]
5	[3, 2]	[2, 1, 1]	[1, 1, 1, 0]	[1, 1, 0, 0, 0]
⋮	⋮	⋮	⋮	⋮
50	[25, 25]	[17, 16, 16]	[12, 12, 12, 12]	[10, 10, 9, 9, 9]

to $n = m-1$, so that there can be m such conditions. The solution for this approximant is $A^{(k)}_{m-1}(\lambda) = \binom{m}{k}(-E_0)^{m-k}$, as can be verified by substitution into (9). It follows that

$$\lambda^m R_{m-1}(\lambda) = [E(\lambda) - E_0]^m. \tag{10}$$

If $n < m-1$ then the resulting approximant cannot be of degree m. However, if we define

$$A^{(k)}_n(\lambda) = \begin{cases} 0 & k > n+1 \\ \binom{n+1}{k}(-E_0)^{n+1-k} & k \leqslant n+1 \end{cases} \tag{11}$$

for $n = -1, 0, 1, \ldots, m-1$, then (9) will be satisfied for all $n \geqslant 0$, with

$$\lambda^{n+1} R_n(\lambda) = [E(\lambda) - E_0]^{n+1}. \tag{12}$$

The following theorem provides recursion relations satisfied by the residuals and by the constituent polynomials.

Theorem 1. Let $\{c_{n,1}, c_{n,2}, \ldots, c_{n,m}\}$ be a set of constants such that

$$R_{n-m-1}(\lambda) + \sum_{j=1}^{m} c_{n,j}\lambda^{j-1} R_{n-m-1+j}(\lambda) = \mathrm{O}(\lambda^m) \tag{13}$$

where the R_k are residuals of degree-m approximants according to (9). Then the constituent polynomials of the diagonal approximant sequence satisfy the recursion

$$A^{(k)}_n(\lambda) = \lambda A^{(k)}_{n-m-1}(\lambda) + \sum_{j=1}^{m} c_{n,j} A^{(k)}_{n-m-1+j}(\lambda) \tag{14}$$

for $n \geqslant m-1$, with $A^{(k)}_n$ at $n < m-1$ given by (11), and the corresponding residuals satisfy

$$\lambda^m R_n(\lambda) = R_{n-m-1}(\lambda) + \sum_{j=1}^{m} c_{n,j}\lambda^{j-1} R_{n-m-1+j}(\lambda) \tag{15}$$

with R_n at $n < m$ given by (12).

Proof. Substitution of (14) into (9) gives

$$\sum_{k=0}^{m} A^{(k)}_n(\lambda) E^k(\lambda) = \lambda^{n-m+1} R_{n-m+1}(\lambda) + \sum_{j=1}^{m} c_{n,j}\lambda^{n-m+j} R_{n-m-1+j}(\lambda) \tag{16}$$

which according to (13) goes to zero asymptotically as $O(\lambda^{n+1})$. Thus, (14) satisfies the accuracy-through-order condition (7), which implies that these $A_n^{(k)}(\lambda)$ are indeed constituent polynomials of the approximant. The fact that the degrees of the polynomials satisfy the index pattern given by (8) can be proved by induction using (14). Comparison of (16) with (9) establishes (15). □

In practice, we calculate the $c_{n,j}$ in the following way (Sergeev 1986). First we define subsidiary residuals $r_p(\lambda)$ according to

$$r_0(\lambda) = R_{n-m-1}(\lambda) \tag{17}$$

$$r_p(\lambda) = \lambda^{-1}[r_{p-1}(\lambda) + c'_{n,p} R_{n-m-1+p}(\lambda)] \tag{18}$$

with

$$c'_{n,p} = -r_{p-1}(0)/R_{n-m-1+p}(0). \tag{19}$$

One can show by induction that

$$\lambda^p r_p(\lambda) = R_{n-m-1}(\lambda) + \sum_{j=1}^{p} c'_{n,j} \lambda^{j-1} R_{n-m-1+j}(\lambda) \tag{20}$$

and that $r_p(\lambda)$ is non-singular at $\lambda = 0$. Comparing (20) for the case $p = m$ with (13) shows that the $c'_{n,j}$ are equal to the $c_{n,j}$. Evaluation of (19) followed by (18) gives a recursive calculation of the $c_{n,j}$ that is convenient to carry out by computer. Comparing (20) with (15) shows that $R_n(\lambda) = r_m(\lambda)$.

It turns out that the $A_n^{(k)}$ generated by this algorithm are normalized so that the leading-order coefficient of $A_n^{(i-1)}$ (i.e. the coefficient multiplying λ^j, with i and j defined by (8)) is equal to 1.

3. Branches of the approximants

Consider the diagonal approximant sequence $E_{\{m,n\}}(\lambda)$, as defined in section 2. These approximants can have as many as m branches, corresponding to the m roots of (6). Let us determine the asymptotic behaviour of these branches at $\lambda \to 0$ and at $\lambda \to \infty$.

It follows from (6) that $E_{\{m,n\}}(0)$ is a root of a polynomial $\mathcal{P}(E_{\{m,n\}}) = \sum_{k=0}^{m} A_n^{(k)}(0) E_{\{m,n\}}^k$. (We do not consider here the case of a multiple root, when $E_{\{m,n\}}(0)$ is also a root of $\mathrm{d}\mathcal{P}/\mathrm{d}E_{\{m,n\}}$, which may occur accidentally but is rare in practice.) According to a theorem of Baker (Baker and Graves-Morris 1995, pp 534–5) the root of equation (6) for which $E_{\{m,n\}}(0)$ is equal to $E(0)$ differs from $\sum_{i=0}^{\infty} E_i \lambda^i$ by an error that is at worst $O(\lambda^{n+1})$. We call this root the *principal branch* and call the sheet of the Riemann surface on which it approximates the function, the *principal sheet*. In general, for all other branches the $\lambda \to 0$ limit of the approximant will not be equal to the $\lambda \to 0$ limit of the asymptotic expansion $\sum_{n=0}^{\infty} E_n \lambda^n$. However, these approximants can, at least in principle, describe the function $E(\lambda)$ on other sheets.

The large-λ behaviour is described by the following theorem.

Theorem 2. Let i be the index defined in (8) that describes the pattern of the degrees of the $A_n^{(k)}$. In the limit $\lambda \to \infty$, $i - 1$ branches of $E_{\{m,n\}}(\lambda)$ tend to constants, while the remaining $m + 1 - i$ branches behave as $\lambda^{1/(m+1-i)}$.

Proof. In the limit $\lambda \to \infty$ the asymptotic behaviour of $E_{\{m,n\}}(\lambda)$ is given by the equation

$$\sum_{k=0}^{i-1} A_{n,0}^{(k)} E_{\{m,n\}}^{k}(\lambda) + \frac{1}{\lambda} \sum_{k=i}^{m} A_{n,0}^{(k)} E_{\{m,n\}}^{k}(\lambda) = 0 \tag{21}$$

where $A_{n,0}^{(k)}$ are the leading-order (i.e. λ^j or λ^{j-1} according to (8)) coefficients of $A_n^{(k)}(\lambda)$. Assume that $E_{\{m,n\}}(\lambda) \sim c\lambda^{\alpha}$, where c and α are constants. We consider three possibilities: $\alpha = 0$, $\alpha > 0$, and $\alpha < 0$. If $\alpha = 0$ then at leading order we have $\sum_{k=0}^{i-1} A_{n,0}^{(k)} c^k = 0$, which has $i - 1$ solutions for c if $i > 1$ and no solutions if $i = 1$. If $\alpha > 0$ then $A_{n,0}^{(m)} c^{m+1-i} \lambda^{(m+1-i)\alpha - 1} - A_{n,0}^{(i-1)} = 0$. This has a solution only if $\alpha = m + 1 - i$. If $\alpha < 0$, then at leading order in λ we have $A_{n,0}^{(0)} = 0$, which has no solution. □

We determine the value of E by solving for a root of (6) using an iterative numerical algorithm. In practice, to ensure convergence to the particular branch of interest, we begin with an estimate of the desired result obtained from some other method as the initial guess for the root.

4. A simple example of a multiple-valued function

Consider the infinite-valued function $F(\lambda) = \lambda^{-1}[\ln(1+\lambda) + 2\pi K \mathrm{i}]$, where K is an integer indicating the branch. For the principal branch, $K = 0$, F has the asymptotic expansion

$$F(\lambda) \sim 1 - \tfrac{1}{2}\lambda + \tfrac{1}{3}\lambda^2 - \tfrac{1}{4}\lambda^3 + \tfrac{1}{5}\lambda^4 - \tfrac{1}{6}\lambda^5 + \cdots. \tag{22}$$

It has been proved (Bender and Orszag 1978 pp 402–3) that the convergence of linear approximants for (22) to the principal branch is geometric. We know of no such theoretical estimates for higher-degree approximants but find numerically that the diagonal sequences of approximants of any degree also converge geometrically, with

$$|F_{\{m,n\}}(\lambda) - F(\lambda)| \propto \left| \frac{1 - (1+\lambda)^{(m+1)^{-1}} \exp\left(\frac{2\pi \mathrm{i}}{m+1}\left[\frac{m+1}{2}\right]\right)}{1 - (1+\lambda)^{(m+1)^{-1}} \exp\left(\frac{2\pi \mathrm{i}}{m+1} K\right)} \right|^n \tag{23}$$

where $[\frac{m+1}{2}]$ is the greatest integer less than or equal to $\frac{m+1}{2}$. It follows that the approximant sequence will converge on those branches for which $|K| \leqslant [\frac{m-1}{2}]$. On such branches, (23) in the limit of large m reduces to

$$|F_{\{m,n\}} - F| \propto [\tfrac{1}{4}\ln^2(1+\lambda) + \pi^2 K^2]^{n/2} m^{-n}. \tag{24}$$

Thus, increasing the degree m always increases the rate of convergence in the limit of large-order n. However, the convergence rate is slower for larger K, corresponding to branches that are more distant from the principal branch.

Of particular interest is the determination of the optimal m for given n. Figure 1 shows the accuracy against m at given values of n for the principal branch and for the $|K| = 2$ branches. In the appendix we develop the following expression for the optimal m:

$$m \approx (n+2)^{1/2} - 1. \tag{25}$$

As shown in figure 1, this expression does in practice give very nearly the highest accuracy.

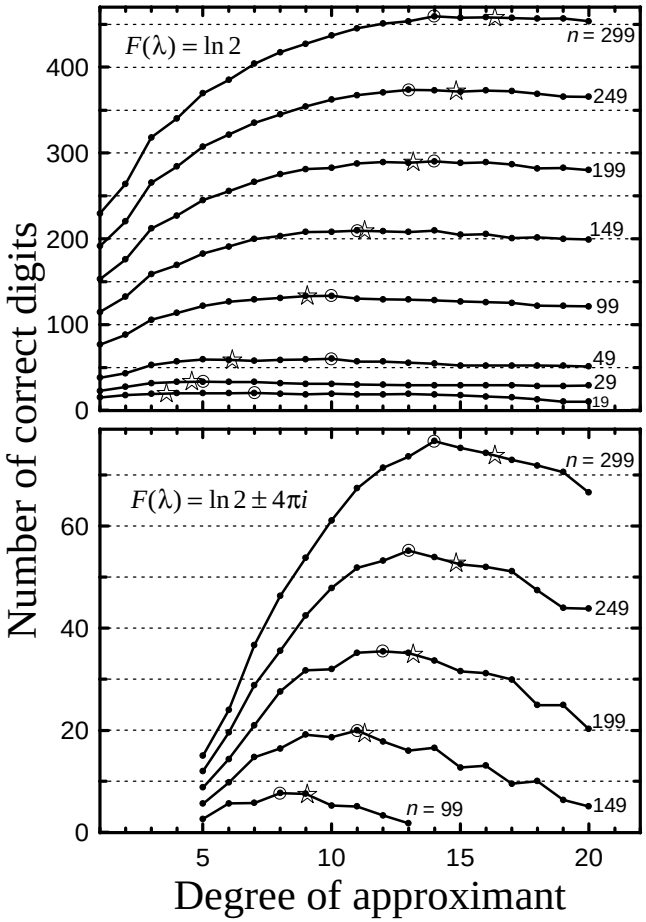

Figure 1. Dependence of accuracy on the degree m of the algebraic approximant of order n in the diagonal staircase sequence for the function $F(\lambda) = \lambda^{-1}[\ln(1+\lambda) + 2\pi \mathrm{i} K]$ on the branches $K = 0$ and $K = \pm 2$ at $\lambda = 1$. The optimal m for given n is indicated by a circle. The predicted optimal m, according to (25) is indicated by a star. The measure of accuracy is $-\lg|F_{\{m,n\}} - F|$, which is roughly equal to the number of correct digits after the decimal point.

5. Anharmonic oscillators

5.1. Quartic oscillator

We have computed the exact asymptotic expansion coefficients for the ground-state energy of the quartic oscillator through 600th order using a linear algebraic method (Vaĭnberg *et al* 1988, Dunn *et al* 1994). The coefficients are rational numbers. Calculations of diagonal staircase approximant sequences were carried out with Mathematica (Wolfram 1991) in multiple-precision arithmetic (5000 digits), because the recursive algorithm is numerically unstable. The accuracy of $E_{\{m,n\}}$ for various λ is shown in figures 2–4.

Figure 2 shows the convergence at $\lambda = \frac{1}{2}$ for the principal branch of $E(\lambda)$, which corresponds to the ground-state energy. The 20th degree approximant sequence appears to converge to 80 decimal digits, which, incidently, surpasses the highest accuracy previously reported for this result, obtained by Meißner and Steinborn (1997) from an iterative

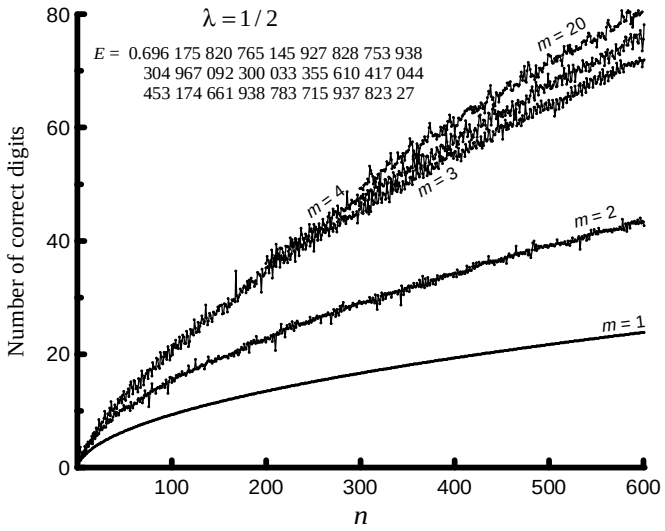

Figure 2. Accuracy of diagonal staircase approximant sequences $E_{\{m,n\}}$ for the ground-state energy of the quartic oscillator at $\lambda = \frac{1}{2}$. n is the order of the perturbation expansion while m is the approximant degree. The measure of accuracy is $-\lg|E_{\{m,n\}} - E|$.

calculation. At large n we find that $\ln|E_{\{m,n\}} - E| \sim -n^{\alpha}$, with the parameter α increasing with m. For $m = 1$ we find numerically that $\alpha = 0.50$, which is the same convergence as linear approximants for the simple Stieltjes series $\sum(-\lambda)^n n!$ (Bender and Orszag 1978 pp 404–5). For $m = 2$, 3, 4, and 20, respectively, we find $\alpha = 0.59$, 0.67, 0.68, and 0.69.

Figure 3 compares the convergence for different λ on the circle $|\lambda| = \frac{1}{2}$. The curves here are polynomial fits, which suppress the relatively small fluctuations around regular trends. Convergence at $\lambda = \mathrm{i}/2$ is similar to that at $\lambda = \frac{1}{2}$, but the accuracy is slightly poorer. (The physical meaning of imaginary coupling constants will be discussed below.) At $\lambda = -\frac{1}{2}$ the potential does not support bound states. Linear approximants no longer converge, but quadratic and, especially, cubic and higher-degree approximants converge fairly well to a complex energy corresponding to a quasistationary state. Using the scaling transformation of the variable $x = x' \exp(-\pi\mathrm{i}/4)$ in the Hamiltonian (1), with $\beta = 4$, one can prove (Crutchfield 1978, Seznec and Zinn-Justin 1978) that $\lambda = \exp(\frac{3}{2}\mathrm{i}\pi)\lambda'$ corresponds to a double-well problem

$$H' = \tfrac{1}{2}p^2 - \tfrac{1}{2}x'^2 + \lambda' x'^4 \tag{26}$$

with eigenvalues $E'(\lambda') = -\mathrm{i}E(\lambda)$. These lie on the second sheet of Riemann surface. The bottom panel of figure 3 corresponds to this branch, with $\lambda' = \frac{1}{2}$.

Figure 4 shows the accuracy of results for $\lambda' = \frac{1}{10}$ and $\lambda' = \frac{3}{100}$. Convergence improves significantly with increasing degree m of the approximant sequences, especially for smaller λ'. We attribute this to the presence on this sheet of the infinite sequence of square-root branch-point pairs, identified by Bender and Wu (1969). The positions of these branch points are shown in figure 5. The closer λ is to these points, the greater is the advantage of increasing the degree of the approximants. $\lambda' = \frac{3}{100}$ corresponds to a λ deep in the heart of the branch-point region. We find that approximants with degree less than 4 do not converge at all at this point while the 20th degree approximants show slow but steady convergence

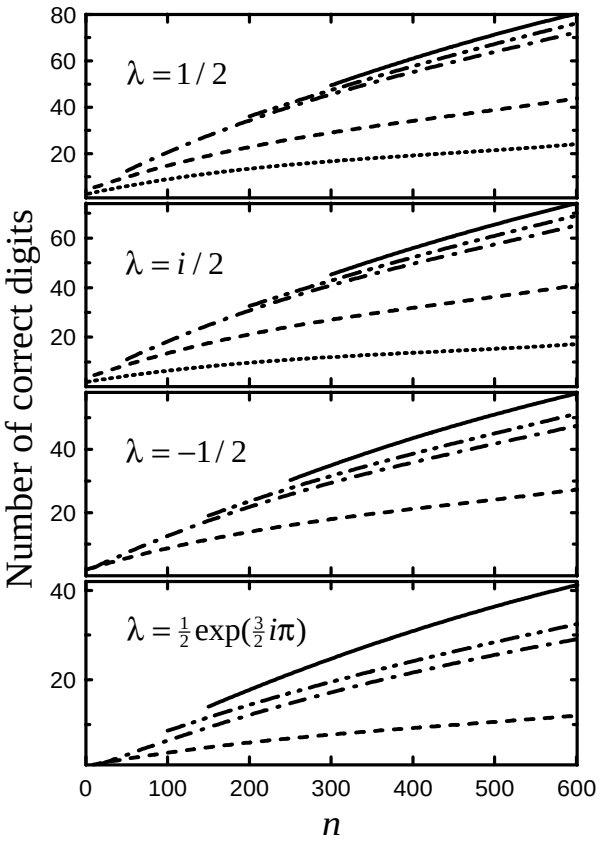

Figure 3. Accuracy of diagonal staircase approximant sequences $E_{\{m,n\}}$ for the ground-state energy of the quartic anharmonic oscillator at different λ on the complex circle $|\lambda| = \frac{1}{2}$. The curves have been smoothed by fitting with a polynomial. The approximant degree is indicated as follows: $m = 1$, $\cdots\cdots$; $m = 2$, $- - -$; $m = 3$, — · —; $m = 4$, — · · —; $m = 20$, ——. The measure of accuracy is $-\lg|E_{\{m,n\}} - E|$. (The vertical scale is different for different λ.)

to a pure imaginary energy,

$$E(\tfrac{3}{100}\mathrm{e}^{3\mathrm{i}\pi/2}) = \mathrm{i}E'(\lambda') = -1.411\,819\,732\,54\mathrm{i} \tag{27}$$

which corresponds to the ground-state energy in the double well. Moreover, another branch of the degree 20 approximants converges (at very high order) to $-0.312\,1621\mathrm{i}$, which corresponds to the energy of the second excited state in the double well. These two branches meet at the branch cut between the first branch points of the sequence, $\pm 0.031\,9934 - 0.036\,7596\mathrm{i}$.

The principal branch of the function $E(\lambda)$ at $\lambda = -\mathrm{i}\lambda'$ corresponds to the complex energy of the barrier resonance in the double well, $E^{\mathrm{r}}_{\mathrm{DW}}(\lambda') = -\mathrm{i}E(-\mathrm{i}\lambda')$. The small-coupling expansion

$$E^{\mathrm{r}}_{\mathrm{DW}}(\lambda') = \frac{-\mathrm{i}}{2} + \frac{3}{4}\lambda' - \frac{21}{8}\mathrm{i}\lambda'^2 + \frac{333}{16}\mathrm{i}\lambda'^3 + \cdots \tag{28}$$

represents a formal Rayleigh–Schrödinger perturbation series for the anharmonic oscillator $\frac{1}{2}\omega^2 x^2 + \lambda' x^4$ with an imaginary frequency $\omega = -\mathrm{i}$. A similar perturbation theory for

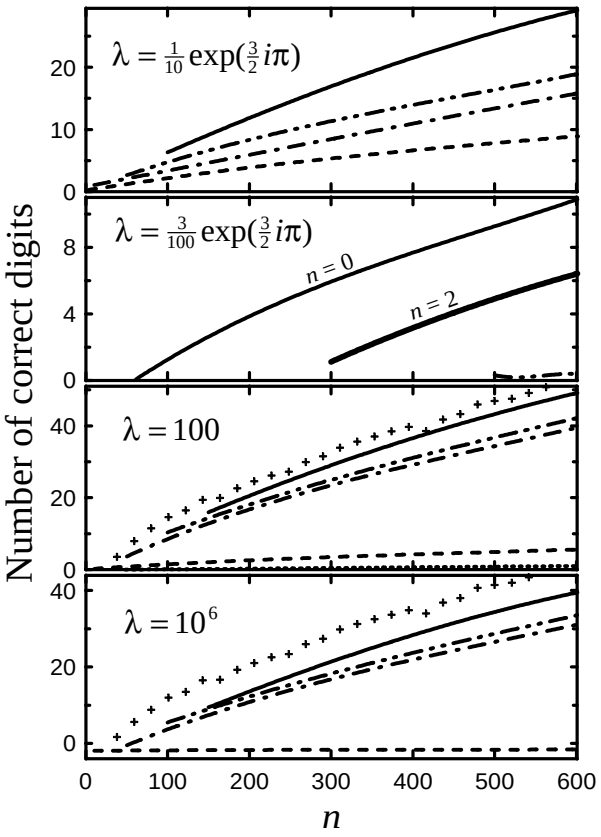

Figure 4. Accuracy of diagonal staircase approximant sequences $E_{\{m,n\}}$ for the ground-state energy of the quartic anharmonic oscillator at various values of λ. The curves are smoothed by polynomial fits. The approximant degree is indicated by curve type as in figure 3. In the bottom two panels approximants that have correct large-λ cube-root behaviour are marked by crosses.

resonances was recently used by Fernández (1996). Such broad resonances with the real part of the energy near the potential maximum are associated with chemical reaction thresholds (Friedman *et al* 1995).

The case $\lambda = -\frac{1}{1000}$ shown in figure 6 corresponds to a quasistationary state with extremely small width, $\Im E \approx \pm 4.319 \times 10^{-144}$. The linear approximants are all pure real. Their error decreases with n until it becomes approximately equal to $|\Im E|$ and then it holds steady at that level. This level of accuracy is eventually reached also by partial summation, just before the divergence sets in. Approximants with $m \geqslant 2$ are real at low n, and their accuracy stalls at the same level as for $m = 1$, but at large n, once an imaginary part appears, the accuracy increases rapidly. This behaviour is qualitatively similar to that observed in a study of molecular resonances with two degrees of freedom using quadratic approximants (Suvernev and Goodson 1997).

The cases $\lambda = 100$ and $\lambda = 10^6$ displayed at the bottom of figure 4 correspond to a strong-coupling region, in which $E(\lambda) \sim b_0\lambda^{1/3}$ (Turbiner and Ushveridze 1988, Guardiola *et al* 1992). Since linear and quadratic approximants cannot accurately model cube-root singularities, their convergence is very slow. Convergence of approximants with $m > 2$ is much better. The 20th degree approximants of the form $[j, j, \ldots, j, j-1, j-1, j-1]$

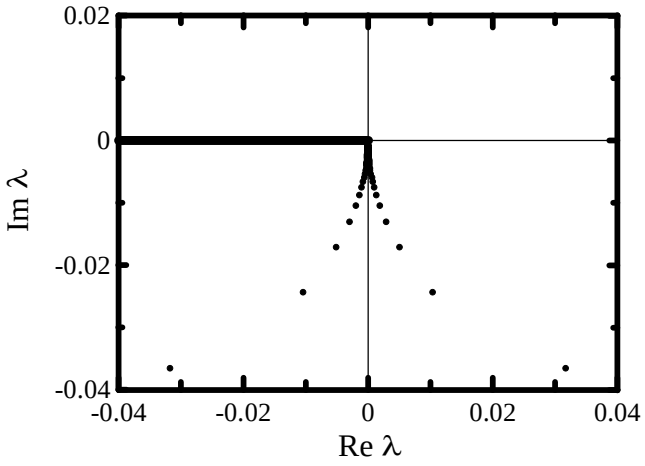

Figure 5. Diagram of analytic structure of $E(\lambda)$ for the quartic oscillator on the second sheet of the Riemann surface corresponding to the branch cut $(0, \infty)$, showing pairs of square root branch points with limit point at the origin (Shanley 1986).

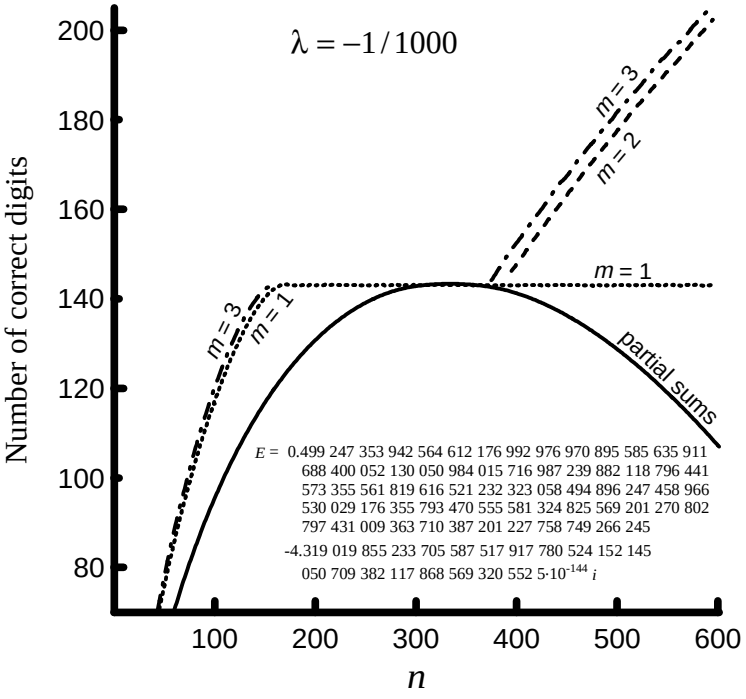

Figure 6. Accuracy of diagonal staircase approximant sequences $E_{\{m,n\}}$ and of partial sums for a very long-lived quasistationary state of the quartic oscillator. Accuracy of approximants with $m > 3$ is indistinguishable from that of cubic approximants within the scale of the figure.

($n = 21j + 16$) are marked by crosses. Their accuracy is significantly higher than the overall accuracy of the 20th degree approximants (full curve) because they always have correct $\lambda^{1/3}$ behaviour at large λ, according to the theorem in section 3.

Apart from dependence of the accuracy on n, we have also studied the dependence on m, that is, the convergence along rows in table 1. The behaviour is qualitatively the same as that in figure 1. The condition (25) gives nearly optimal convergence.

5.2. Cubic oscillator

The harmonic oscillator with cubic perturbation, $H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + gx^3$, is a prototypical system exhibiting resonances. Its complex eigenvalues have been studied numerically (Drummond 1981) and analytically (Alvarez 1988, 1995). One can expect in general that harmonic oscillators with polynomial perturbations of any degree greater than 2 will have an infinite sequence of square-root branch points approaching the origin, and therefore should benefit from the use of high-degree approximants.

Since odd-order terms of the energy series in g are zero (because the energy is an even function of g), we define the perturbation parameter as $\lambda = g^2$ and analyse the series $E(\lambda) \sim \frac{1}{2} - \frac{11}{8}\lambda - \frac{465}{32}\lambda^2 - \cdots$, which has non-zero terms at every order. Convergence of the algebraic approximants for $\lambda = \frac{1}{4}$ (i.e. $g = \frac{1}{2}$), $\lambda = \frac{1}{4}\exp(5\mathrm{i}\pi/2)$, and $\lambda = 100$ is shown in figure 7. The convergence behaviour is quite similar to that for the quartic oscillator. However, for the quartic oscillator, which has a cube-root branch structure, there was significant improvement from increasing m up to 3 and more modest improvement for $m > 3$. For the cubic oscillator, with a fifth-root structure (Alvarez 1995), there is a greater advantage from increasing m above 3. This is especially true for the large-λ case, shown in the bottom panel, where the asymptotic $\lambda^{1/5}$ behaviour becomes dominant in $E(\lambda)$. For the $m = 20$ case the accuracy of approximants of the form $[j, \ldots, j, j-1, j-1, j-1, j-1, j-1]$ is marked by crosses. Their accuracy is consistently higher than the average accuracy of the $E_{\{20,n\}}$, as expected from the theorem in section 3.

Using the scaling transformation $x = \omega^{1/2}x'$, one can prove that $\omega E(\omega^{-5}\lambda)$ is an eigenvalue in a potential $\omega^2x^2/2 + \lambda^{1/2}x^3$. In particular, for $\omega = \exp(-\pi\mathrm{i}/2)$, the value $-\mathrm{i}E(\mathrm{e}^{\frac{5}{2}\mathrm{i}\pi}\lambda)$ is an eigenvalue in a potential $-x^2/2+\lambda^{1/2}x^3$. A shift transformation transforms this modified potential back to the original potential,

$$-\tfrac{1}{2}x^2 + \lambda^{1/2}x^3 = \tfrac{1}{2}x'^2 + \lambda^{1/2}x'^3 - 1/(54\lambda) \tag{29}$$

where $x' = x + 1/(3\lambda^{1/2})$, which implies that the eigenvalues $E(\lambda)$ in the original potential can be expressed in terms of the new eigenvalues according to

$$E(\lambda) = -\mathrm{i}E(\lambda') + 1/(54\lambda) \tag{30}$$

where $\lambda' = \exp(\frac{5}{2}\mathrm{i}\pi)\lambda$. The point λ' lies on the second sheet of the Riemann surface under the cut $(0, \infty)$. $E(\lambda')$ can be expressed as $E'(\mathrm{i}\lambda)$ where E' represents the second branch of the function E. Thus, the eigenvalues can be calculated either by direct summation of the series $E(\lambda)$ on the principal sheet or by summing the expansion for E' on its second sheet. The latter approach is equivalent to expanding the potential $-x^2/2 + \lambda^{1/2}x^3$ at its local maximum and then developing a complex perturbation theory for an upturned oscillator with pure imaginary frequency with summation of the energy expansion on the second sheet. As shown in the second panel of figure 7, this indirect approach does indeed converge to the same result as the direct approach, and it benefits even more strongly from the use of high-degree approximants, although the rate of convergence appears to always be less than that of the direct analysis.

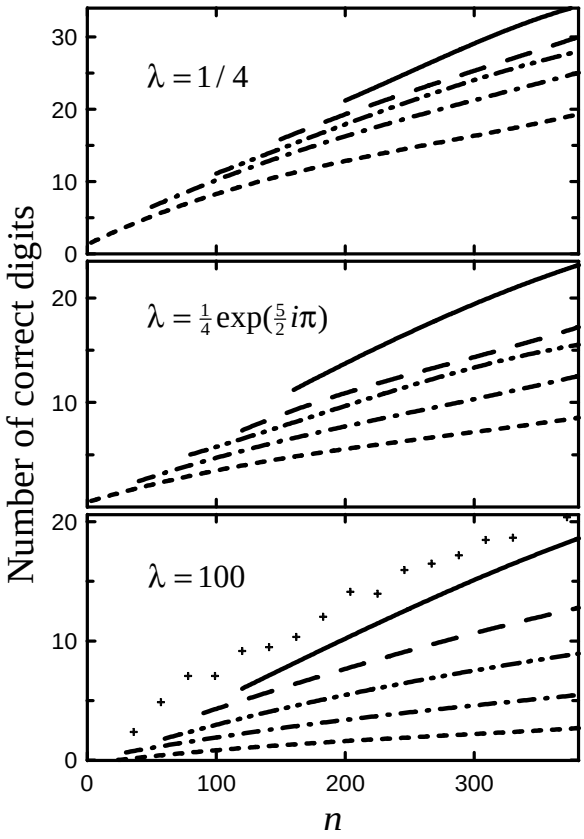

Figure 7. Accuracy of diagonal staircase approximant sequences $E_{\{m,n\}}$ for the ground state energy of the cubic anharmonic oscillator at different values of λ. The curves are smoothed by polynomial fits. The approximant degree is indicated by curve type as in figure 3. The energy at $\lambda = \frac{1}{4}\exp(\frac{5}{2}i\pi)$ is closely related to the energy at $\lambda = \frac{1}{4}$ according to (30). In the bottom panel approximants that have correct large-λ fifth-root behaviour are marked by crosses.

5.3. Sextic and octic oscillators

Perturbation theory for sextic (λx^6) and octic (λx^8) anharmonic oscillators is very strongly divergent—the E_n grow as $(2n)!$ and $(3n)!$, respectively. Linear approximants converge very slowly for the sextic oscillator even at small λ and fail to converge at all for the octic oscillator (Graffi and Grecchi 1978). Figure 8 shows that increasing the approximant degree for the sextic oscillator considerably improves the convergence rate.

The problem of the octic oscillator is particularly interesting because the $[j, j]$ and $[j+1, j]$ sequences of linear approximants converge to different limits, giving lower and upper bounds to the true energy (Austin 1984). We find that higher-degree approximants of a given index pattern also converge to an incorrect result but the number of digits of agreement with the correct result is considerably greater than that for linear approximants. This behaviour is shown in figure 9 for diagonal quadratic and cubic approximants. The accuracy obtained both for the sextic and for the octic oscillator exceeds the accuracy obtained by Weniger *et al* (1993) using a nonlinear transformation of a renormalized series.

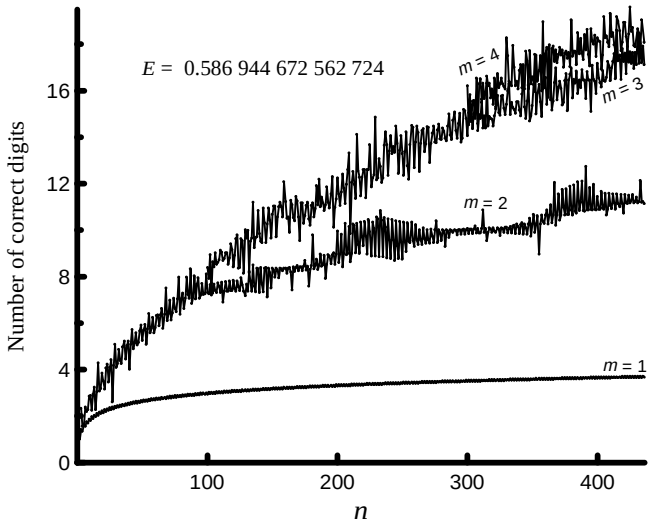

Figure 8. Accuracy of diagonal staircase approximant sequences $E_{\{m,n\}}$ for the ground state energy of the sextic oscillator at $\lambda = \frac{1}{10}$.

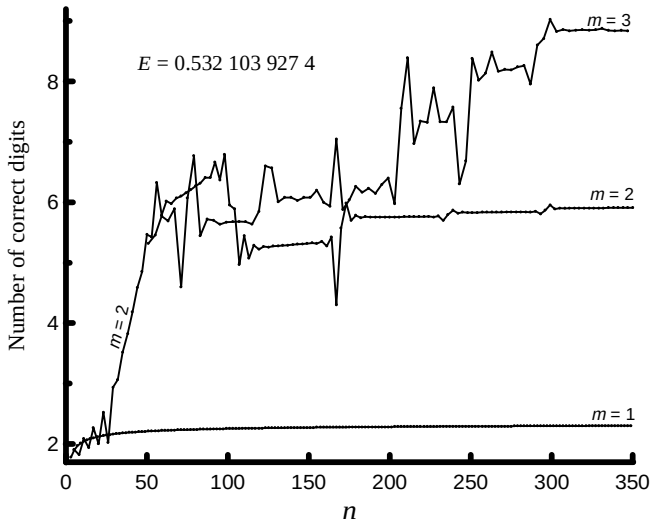

Figure 9. Accuracy of diagonal approximants $E_{[j,j,\ldots,j]}$ for the ground state energy of the octic oscillator at $\lambda = \frac{1}{100}$, with approximant degree m as indicated. The linear approximants converge to 0.5272 (99.1% of the exact energy), the quadratic approximants converge to 0.532 105 (100.0002%), and the cubic approximants converge to 0.532 103 926 (99.999 9997%). The 'exact' energy for this system was calculated by numerical integration of the differential equation.

6. Conclusions

We have demonstrated that algebraic approximants of degree $m \geqslant 3$ can be very effective for summing perturbation series for quantum oscillators, both on the principal sheet and on nearby sheets of the Riemann surface. These approximants can reproduce several sheets of a multiple-valued function starting from the Taylor expansion of the function on the

principal sheet. The eigenvalues of a given symmetry are branches of a single multiple-valued function and the branch points form a sequence with the limit point at the origin. Similar singularity structure has also been identified for other kinds of potentials, including the angular spheroidal wave equation (Hunter and Guerrieri 1982), the two-centre Coulomb problem (Grozdanov and Solov'ev 1990), and analytically solvable models (Bender *et al* 1974, Ushveridze 1988). To the extent that such structure is typical of quantum mechanical eigenvalues, we expect that algebraic approximants will be useful as a general summation method for perturbation theories of the Schrödinger equation.

We expect that the accuracy of our results could be improved by applying the approximants to expansions calculated from renormalized Hamiltonians (Killingbeck 1981, Arteca *et al* 1990 pp 126–31, Vinette and Čížek 1991, Weniger *et al* 1993). For example, Weniger (1996) obtained an accuracy of 46 digits from 198th order perturbation theory for the ground-state energy of the quartic oscillator with $\lambda = \frac{1}{2}$, using a sequence transformation to sum a renormalized expansion. This rate of convergence is somewhat better than that reported here in figure 3.

A limitation of algebraic approximants is that in practice the number of expansion coefficients needed for a given degree is approximately equal to the square of the degree. Therefore, approximants of very high degree will be most useful for problems with few degrees of freedom, for which the perturbation theory can be computed to very high order.

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Appendix. Predicting the optimal degree

The defining relation for algebraic approximants of the function $E(\lambda)$, which we have written in (7) as a polynomial in E, can also be thought of as a polynomial equation in terms of λ. Thus, if we substitute the explicit expression $\sum_{i=0}^{p_k} a_{k,i}\lambda^i$ for $A^{(k)}$, then we can write (7) in the form

$$\sum_{i=0}^{q} B^{(i)}(E)\lambda^i = \mathrm{O}(\lambda^{n+1}) \tag{A1}$$

in terms of a set of polynomials $B^{(i)}$, with $q = [(n+1)/(m+1)]$. It follows that (7) simultaneously defines an algebraic approximant of degree m for $E(\lambda)$ and algebraic approximant of degree q for the inverse function $\lambda(E)$.

In principle, if $E(\lambda)$ has an infinite number of branches then we can expect that the accuracy of the approximant $E_{\{m,n\}}$ will increase with m. However, the error in the approximant $E_{\{m,n\}}$ is related to the error in the approximant $\lambda_{\{q,n\}}$. Let

$$\delta E = E(\lambda_s) - E_{\{m,n\}}(\lambda_s) \qquad \delta\lambda = \lambda(E_s) - \lambda_{\{q,n\}}(E_s) \tag{A2}$$

where λ_s is the point at which E is being summed and $E_s = E(\lambda_s)$. Then $E_{\{m,n\}}(\lambda_s) = E_{\{m,n\}}(\lambda(E_s) + \delta\lambda)$. Assuming that $\delta\lambda$ is small, it follows that

$$E_{\{m,n\}}(\lambda_s) \approx E_s + \delta\lambda\frac{\mathrm{d}E_{\{m,n\}}}{\mathrm{d}\lambda} \approx E_s + \delta\lambda\frac{\mathrm{d}E}{\mathrm{d}\lambda} \tag{A3}$$

which implies that δE is proportional to $\delta\lambda$. Let us assume that $\lambda(E)$ is a multiple-valued function. (This is true for our model function $x^{-1}\ln(1+x)$.) Then we can expect that the accuracy of the approximants $\lambda_{\{q,n\}}$ will increase with q. However, q decreases with m. This implies that the accuracy of $E_{\{m,n\}}$ will *decrease* with m.

Thus, we need m somewhat large, to model the singularity structure of $E(\lambda)$, but we also need q somewhat large, to model the singularity structure of $\lambda(E)$. Based on these arguments, we conjecture that the optimal approximant degree will correspond to $m \approx q$, from which (25) follows.

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