On the extrapolation of perturbation series

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Abstract. We discuss certain special cases of algebraic approximants that are given as zeroes of so-called effective characteristic polynomials and their generalization to a multiseries setting. These approximants are useful for the convergence acceleration or summation of quantum mechanical perturbation series. Examples will be given and some properties will be discussed.

Keywords: Convergence acceleration, Extrapolation, Summation of divergent series, Effective characteristic polynomials, Algebraic approximants, Multiseries approximants, Quantum mechanics, Perturbation theory, Anharmonic oscillators

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1. Introduction

In quantum mechanics, the usual Rayleigh-Schrödinger Perturbation Theory (RSPT) is used for solving the eigenvalue problem of a Hamilton operator

\[ H = H_0 + \beta V \]

in terms of an unperturbed Hamiltonian \( H_0 \) with known spectrum, a perturbation \( V \) and a coupling constant \( \beta > 0 \). The RSPT yields for the \( I \)-th eigenvalue a formal power series

\[ E^{(I)}(\beta) = E_0^{(I)} + \beta E_1^{(I)} + \ldots + \beta^n E_n^{(I)} + \ldots \]

with real coefficients \( E_n^{(I)} \). Such series are often divergent, for instance for the quartic anharmonic oscillator (AHO) with Hamiltonian

\[ H = -\frac{d^2}{dx^2} + x^2 + \beta x^4 \]

on the real line. For this and closely related problems, there is a vast amount of literature since the quartic AHO may be considered as

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the prototype of a zero-dimensional $\Phi^4$ field theory, and thus, it has been used as test case for almost every important numerical method to solve the quantum mechanical eigenvalue problem. A recent example is the use of the generalized Bloch equation as an iterative method for the solution of the Schrödinger equation [18, 14, 20]. For the quartic AHO, the $n$-th term $a_n$ in the RSPT series behaves as $a_n \sim -\sqrt{24/\pi^3}(-3\beta/2)^n\Gamma(n+1/2)$ for large $n$ [3, 4, 5] and the series has zero radius of convergence in the variable $\beta$. Thus, one has to sum such alternating divergent series.

There are many summation methods that can be used in principle, a review of which is outside the scope of the present article. Consider a (formal) power series

$$f(\beta) = \sum_{j=0}^{\infty} c_j \beta^j$$

with partial sums

$$s_n = \sum_{j=0}^{n} c_j \beta^j .$$

An important class of summation methods are nonlinear sequence transformations that transform the sequence $\{s_n\}_{n=0}^{\infty}$ of partial sums to a new transformed sequence $\{s'_n\}_{n=0}^{\infty}$ that is assumed to converge to the so-called antilimit of the divergent sequence $\{s_n\}$. This antilimit is taken as the result of the summation process.

We mention some examples of nonlinear sequence transformations. One is the famous epsilon algorithm [31] It computes the upper half of the Padé table for the power series $f(\beta)$ according to [23, 31]

$$\epsilon_{2k}^{(n)} = \left[ n + k / k \right], \quad (k \geq 0, n \geq 0).$$

(6)

Additionally, the epsilon algorithm is related to the Shanks transformation [23]. Unfortunately, the epsilon algorithm is unable to sum several important perturbation series, for instance the RSPT series for the ground state of the octic anharmonic oscillator [29].

As a second nonlinear sequence transformation, we mention the $S$ transformation of Weniger [28, Sec. 8] that may be defined by the recursive scheme

$$\tilde{D}_n^{(0)} = 1/\omega_n ,$$

$$\tilde{N}_n^{(0)} = s_n/\omega_n ,$$

$$\tilde{D}_n^{(k)} = \tilde{D}_{n+1}^{(k-1)} - \Psi_n^{(k-1)}\tilde{D}_n^{(k-1)}, \quad (k \geq 1) ,$$

$$\tilde{N}_n^{(k)} = \tilde{N}_{n+1}^{(k-1)} - \Psi_n^{(k-1)}\tilde{N}_n^{(k-1)}, \quad (k \geq 1) ,$$

(7a)  
(7b)  
(7c)  
(7d)
\[ \frac{N_n^{(k)}}{D_n^{(k)}} = S_n^{(k)}(\zeta, \{s_n\}; \{\omega_n\}) \]  \hfill (7e)

with [28, Sec. 8.3]

\[ \Psi_n^{(k)} = (\zeta + n + k)(\zeta + n + k - 1) \over (\zeta + n + 2k)(\zeta + n + 2k - 1) \]  \hfill (8)

The \( S \) transformation depends on an auxiliary sequence \( \{\omega_n\}_n^{\infty} \) of \textit{remainder estimates} with \( \omega_n \neq 0 \). Several variants for the choice of the latter may be considered [16, 13, 7]. For the choice \( \omega_n = s_{n+1} - s_n \), originally proposed by Smith and Ford [26], one obtains the \( \tilde{t} \) variant (or \( d \) variant in the notation of Weniger [28]), i.e.,

\[ \tilde{t} S_n^{(k)}(\zeta, \{s_n\}) = S_n^{(k)}(\zeta, \{s_n\}, \{s_{n+1} - s_n\}) \]  \hfill (9)

Eq. (7) is essentially one of the recursive schemes for the computation of the \( J \) transformation which is a rather general and well-studied sequence transformation that covers many of the most successful transformations as special cases [8, 9, 10, 11, 13, 15, 7]. The particular choice (8) corresponds to the fact that the \( S \) transformation is identical to a special case of the \( J \) transformation, namely the case \( p = 3 \) of the \( p \)J transformation [1, 11, 7].

Numerical comparison of results of the summation of the RSPT series for the ground state of the quartic AHO using the epsilon algorithm and the \( \tilde{t} \)-variant of the \( S \) transformation shows that the \( S \) transformation is more powerful than the epsilon algorithm for the summation of this particular perturbation series that is rather strongly divergent. [29]

An important additional consideration stems from regarding the perturbation series as function for complex \( \beta \), i.e., one considers an analytic continuation of the formal power series to a function in the complex plane. Then, in principle, one has to allow for several branches of such a function. This question was studied intensively for the quartic AHO by Bender and Wu [3, 4, 5] and Simon [24, 25]. \( E(\beta) \) has a third-order branch point at \( \beta = 0 \) that dominates the behavior for large \( \beta \), i.e., \( E(\beta) = O(\beta^{1/3}) \) for \( \beta \rightarrow \infty \). In the case of AHOs, often renormalized series are used that correspond — up to a factor — to a reexpansion of the original series in a transformed variable \( \kappa \). The relation between \( \kappa \) and \( \beta \) for the quartic AHO may be obtained using Symanzik scaling \( x \rightarrow (1 - \kappa)^{1/4}x \) plus a certain minimization criterion to be [25, 30]

\[ \beta = \frac{\kappa}{3(1 - \kappa)^{3/2}} \]  \hfill (10)
After renormalization, one has to consider a Hamiltonian $\hat{H}(\kappa) = \hat{H}_0 + \kappa \hat{V}$ with an unperturbed Hamiltonian $\hat{H}_0 = -d^2/dx^2 + x^2$ and a perturbation $\hat{V} = (x^4 - 3x^2)/3$. Further, the eigenvalues of $\hat{H}(\kappa)$ and $\hat{H} = H(\beta)$ are related by $\tilde{E}(\kappa) = (1 - \kappa)^{1/2} E(\beta)$. Besides making the renormalized expansion less divergent, the effect of such a renormalization is that the interval $(0, \infty)$ for $\beta$ corresponds to a finite interval, e.g., to $(0, 1)$ for $\kappa$.

Thus, $E(\beta)$ is a multiple-valued function for complex $\beta$ [24, 25]. This type of analytic structure is not easy to simulate using rational approximants in $\beta$ that result on applying either the epsilon algorithm or the $S$ transformation (or other Levin-type sequence transformations [7]) to the RSPT series in $\beta$ of $E(1, \beta)$. Such a behavior of $E(1, \beta)$ can much easier be approximated by algebraic functions in $\beta$ instead of rational functions. These algebraic functions are nothing but zeroes of polynomials with coefficients that depend on $\beta$. For AHOs, this seemingly first was recognized by Cizek and coworkers who considered polynomials of a special structure, the so-called effective characteristic polynomials and applied these to sum the divergent AHO RSPT series [6]. Effective characteristic polynomials have also been applied successfully for the extrapolation of quantum chemical many-body perturbation series [12] and been proven to be size-extensive, i.e., to scale correctly with the particle number [14] in this context. Later, Sergeev and Goodson [21] used more general polynomials that give rise to algebraic approximants [2, Sec. 8.6] for the summation of the ground state of AHOs. Algebraic approximants are generalizations of the quadratic approximants introduced by Shafer [22]. These types of algebraic approximations will be discussed more thoroughly in later sections.

All the methods mentioned above and most other methods for the summation of divergent perturbation series only use the partial sums or the coefficients of a single series, i.e., the RSPT series of one eigenvalue for a particular value of the coupling constant $\beta$. The rest of the methods may be classified as multipoint or multiseries methods.

Multipoint methods are those where still a single eigenvalue $E(I)(\beta)$ is approximated but several Taylor expansions at different points $\beta_i$ are combined to construct the approximation. The most prominent example for such methods are multipoint Padé approximants [2]. It should be noted that the large-coupling regime $\beta \to \infty$ corresponds to $\kappa \to 1$ in the renormalized treatment and can be included in a multipoint treatment. For instance, Cizek and coworkers used two-point Padé approximants for this purpose [6]. For details of such an approach, the reader is referred to the literature, e.g. Refs. [1, 22].
Extrapolation of Perturbation Series

In the present work, we consider multiseries methods. These are different from multipoint methods since the aim is to approximate several functions depending on $\beta$ simultaneously using their Taylor series at a common point, e.g., $\beta = 0$. This multiseries problem occurs naturally in quantum mechanical eigenvalue problems since the Hamilton operator normally possesses several discrete eigenvalues. Using the same splitting of the Hamiltonian in unperturbed operator and perturbation involving the same coupling constant $\beta$ for all these eigenvalues considered as functions of $\beta$, it is clear that the RSPT series of the form (2) for several values of $I$ are not independent. In the context of rational approximation, this multiseries problem leads to simultaneous Padé approximants [3, Sec. 8.1] or vector Padé approximants [3, Sec. 8.4]. On the other hand, combining the idea of a multiseries method and the approximation by algebraic functions, it is rather natural to construct a polynomial with coefficients that depend on $\beta$ by using the coefficients of several perturbation series simultaneously [13]. The resulting algebraic approximations are called *polynomial-type multiseries approximants* and are the main topic of the present article. These are related to, but different from Hermite-Padé approximants as is explained later.

The possible combination of the multipoint and the multiseries concepts leading to the construction of multipoint multiseries approximants is not considered in the present work.

The outline of the article is as follows. First, we will discuss the relation between effective characteristic polynomials and algebraic approximants. Then, multiseries approximants are introduced and several special types of these approximants are defined. Some properties of multiseries approximants are derived. In the last section, numerical test results for the case of the unrenormalized quartic AHO are presented.

2. Effective Characteristic Polynomials

In this section, we sketch effective characteristic polynomials and some of their properties that are known in the literature, and point out that they are special cases of algebraic approximants. Also, the aim is to motivate the extension to a multiseries setting discussed in later sections.

Consider a polynomial of degree $N$ in $E$ with coefficients that are polynomials in $\beta$ of the form

$$P_N(E) = \sum_{j=0}^{N} E^j \sum_{k=0}^{N-j} f_{N,j,k} \beta^k, \quad f_{N,N,0} = 1.$$  

(11)
Such a polynomial depends on $(N + 3)N/2$ coefficients $f_{N,j,k}$ and is called an effective characteristic polynomial \[6, 12, 14\]. The reason for the nomenclature is that characteristic polynomials of this form arise in the linear variational method in an orthonormal basis $\phi_j$, $j = 1, \ldots, N$ for Hamiltonians $H = H_0 + \beta V$, and usually, the $f$'s are computed via matrix elements of $H$ in this basis. For effective characteristic polynomials, however, the $f$'s are obtained from a perturbation series

$$E(\beta) = \sum_{j=0}^{\infty} E_j \beta^j$$  \hspace{1cm} (12)

by requiring that

$$P_N(E(\beta)) = O(\beta^{N(N+3)/2})$$  \hspace{1cm} (13)

holds for $\beta \to 0$. This leads to a system of linear equations for the $f$'s with as many equations as there are unknowns. If this system possesses a solution, the $f$'s and thus, the effective characteristic polynomials are uniquely defined. For known $f$'s, the eigenvalues are approximated by zeroes of $P_N$ that are denoted by $\Pi_{N,j}$, $j = 1, \ldots, N$ and are called effective characteristic polynomial approximants. The branch that reproduces the input data is simply denoted by $\Pi_N$ and called the physical branch. In order to discuss the dependence of the approximants on the coefficients $E_j$ of the series (12), the explicit notation $\Pi_{N,j}[E_0, \ldots, E_M]$ is used where $M = N(N + 3)/2 - 1$.

It should be noted that the physical branch can become complex. Then, for $N = 2$ both branches yield complex results, for instance. This, of course, is not reasonable for the computation of discrete eigenvalues of the Hamiltonian that is a self-adjoint operator, and indicates a breakdown of the perturbative approach. Complex values of the approximants, however, make sense for the description of resonances or tunneling processes \[1, \text{Chap. 8}, \text{17}\], and thus, there are problems where the possibility of obtaining complex approximations from real perturbation series is a desired feature.

We now discuss some properties of these approximants. Note that equivalence and invariance properties of algebraic approximants are known from the literature \[4, \text{Sec. 8.6}\] and this is relevant since the latter approximants are generalizations of effective characteristic polynomial approximants as discussed below.

As shown independently in the literature \[12, 14\] before the connection to algebraic approximants was recognized, the effective characteristic polynomial approximant $\Pi_2$ is invariant under a repartitioning of the Hamiltonian where $H_0$ is replaced by the new unperturbed operator $(1 - \alpha)H_0$ and $\alpha$ is some constant. Denoting the corresponding
coefficients of the RSPT eigenvalue series by \( E_j(\alpha) \), one has

\[
\Pi_2[E_0, \ldots, E_4] = \Pi_2[E_0(\alpha), \ldots, E_4(\alpha)].
\]

This means that the approximant is invariant under the reparation as the true eigenvalue has to be. In Ref. [14] it is shown that a particular effective characteristic polynomial approximant \( \Pi_{N,j} \) for some \( N \) and \( j \) with \( 1 \leq j \leq N \) has the scaling property

\[
\Pi_{N,j}[c E_0, \ldots, c E_M] = c \Pi_{N,j}[E_0, \ldots, E_M].
\]

This is important to guarantee size-extensitivity, i.e., correct scaling with particle number in many-body perturbation theory [14].

We now show that effective characteristic polynomial approximants are special \textit{algebraic approximants}. These are generalizations of Padé approximants. Algebraic approximants are constructed via polynomials \( A^{(k)} \) in \( \beta \) with \( \text{deg}(A^{(k)}) = d_k \), \( k = 0, \ldots, N \) such that for \( Q = -1 + N + \sum_{k=0}^{N} d_k \) and for a given power series \( E(\beta) \) as defined in Eq. (12) the relations

\[
P_N(E(\beta)) = \sum_{k=0}^{N} A^{(k)}(\beta)[E(\beta)]^k = O(\beta^{Q+1})
\]

are satisfied for \( \beta \to 0 \). Since this defines the polynomials only up to a common factor, we additionally demand \( A^{(N)}(0) = 1 \) as a normalization. For given polynomials \( A^{(k)} \), the algebraic approximants \( E_{[d_0,d_1,\ldots,d_N],j} \) are defined as the zeroes of the polynomial \( P_N \) according to

\[
P_N \left( E_{[d_0,d_1,\ldots,d_N],j} \right) = 0, \quad (j = 1, \ldots, N),
\]

and depend on \( Q + 1 \) coefficients \( E_0, \ldots, E_Q \) that play the role of the input data. Again, one may define the physical branch as that one which reproduces the input data via a Taylor expansion in \( \beta \).

Comparison with the definition of effective characteristic polynomial approximants reveals that the latter are nothing but the special algebraic approximants

\[
\Pi_{N,j} = E_{[N,N-1,N-2,\ldots,0],j}, \quad (j = 1, \ldots, N).
\]

It should be noted that algebraic approximants

\begin{itemize}
  \item are special cases of Hermite-Padé approximants and are described by a quite elaborate mathematical theory [2, Sec. 8.5, 8.6]
  \item are useful for multi-valued functions (analytic continuation to another Riemann sheet)
\end{itemize}
have been applied successfully to anharmonic oscillators \cite{21} as noted in the introduction.

3. Polynomial-type Multiseries Approximants

In this section, we define the polynomial-type multiseries approximants, and introduce three special cases (Π-, D-, and P-type approximants). The relation to Hermite-Padé approximants is pointed out. An example is given for Π-type approximants. Further, it is proved that the polynomial coefficients of P-type approximants can be computed recursively.

As indicated in the introduction, the key idea of the present work is to use coefficients of several perturbation series for different eigenvalues to compute the algebraic approximants.

For the definition of \textit{polynomial-type multiseries approximants}, we consider a polynomial

\[
P_N(z) = \sum_{k=0}^{N} A^{(k)}(\beta) z^k
\]

(19)

where the coefficients \(A^{(k)}\) are polynomials in \(\beta\) with \(\deg(A^{(k)}) = d_k \geq 0\) for \(k = 1, \ldots, N\). They satisfy for \(\beta \to 0\) the order conditions

\[
P_N(E^{(I)}(\beta)) = O(\beta^{Q_I+1}), \quad (I = 1, \ldots, S)
\]

(20)

for \(S\) given series \(E^{(I)}(\beta)\) of the form \(\text{[2]}\) and \(S\) parameters \(Q_I\) restricted by demanding

\[
\sum_{I=1}^{S} (Q_I + 1) = N + \sum_{k=0}^{N} d_k.
\]

(21)

The normalization condition is \(A^{(N)}(0) = 1\). The latter and the order conditions \(\text{[21]}\) again lead to a system of linear equations for the coefficients of the polynomials \(A^{(k)}\) with as many unknowns as equations if \(\text{[21]}\) is satisfied. Hence the polynomials \(A^{(k)}\) are uniquely defined if the linear system possesses a solution as is assumed in the following.

Given the polynomials \(A^{(k)}\), the multiseries approximants \(E_{[d_0,d_1,\ldots,d_N],j}^{[Q_1,\ldots,Q_S]}\) are defined as the zeroes of \(P_N\), i.e.,

\[
P_N \left( E_{[d_0,d_1,\ldots,d_N],j}^{[Q_1,\ldots,Q_S]} \right) = 0.
\]

(22)

\footnote{These are called simply multiseries approximants in the following.}
These approximants depend on $\beta$ and the coefficients
\[ E_I^{(I)}, \ldots, E_Q^{(I)}, \quad I = 1, \ldots, S. \] (23)

We are especially interested in the case that $S = N$ which means that as many perturbation series are used as there are roots of $P_N$, i.e., as there are approximants. In this case, the consistency condition becomes
\[ \sum_{I=1}^{N} Q_I = \sum_{k=0}^{N} d_k. \] (24)

Therefore, we define the following special cases:

**Π-type approximants with** $S = N$
\[ \Pi^{[N],j} = E^{[N,N-1,N-2,\ldots,1]}_{[N,N-1,N-2,\ldots,1],j}, \quad (j = 1, \ldots, N). \] (25)

Here, Eq. (24) is obviously satisfied.

**D-type approximants with** $S = N$ for even $N = 2D$
\[ D^{[N],j} = E^{[N,N-1,N-2,\ldots,1]}_{[D,\ldots,D],j}, \quad (j = 1, \ldots, N). \] (26)

Here, Eq. (24) is satisfied: The left hand side is $N(N + 1)/2$, the right hand side is $D(N + 1)$, and both agree since $N = 2D$.

**P-type approximants with** $S = N$
\[ P^{[Q],j} = E^{[Q,Q,\ldots,Q]}_{[Q,Q,\ldots,Q],0,j}, \quad (j = 1, \ldots, N). \] (27)

Here again, Eq. (24) is obviously satisfied.

Π-type approximants were introduced by the author [13], D- and P-type approximants are new.

We note that these multiseries approximants
– are related to, but different from Hermite-Padé approximants [2, Sec. 8.5]. To be more specific, we remark that the order conditions (20) are different from those satisfied by the Hermite-Padé polynomials $a_{I,m_I}(\beta)$ that are constructed from the same $S$ power series $E^{(I)}(\beta), I = 1, \ldots, S$ via, e.g.,
\[ a_{I,0}(\beta) + \sum_{I=1}^{S} \sum_{m_I=1}^{M_I} a_{I,m_I}(\beta)[E^{(I)}(\beta)]^{m_I} = O(\beta^\tau) \] (28)

for suitable $M_I$ and $\tau$. This should be compared to Eqs. (19) and (27).
are useful for multi-valued functions (analytic continuation to another Riemann sheet),

- have no convergence theory so far, and

- are possibly cheaper than algebraic approximants since the numerical effort to compute several short perturbation expansions is much less than one long expansion.

As a simple example, we consider the harmonic oscillator problem with Hamiltonian

\[ H = -\frac{d^2}{dx^2} + (1 + \beta)x^2, \quad H_0 = H - \beta x^2 \]  

with eigenvalues

\[ E^{(I)} = (2I - 1)\sqrt{1 + \beta}. \]  

The coefficients of the perturbation series follow by Taylor expansion of the \( E^{(I)} \):

\[ E^{(1)} = 1 + \frac{1}{2}\beta - \frac{1}{8}\beta^2 + \frac{1}{16}\beta^3 - \frac{5}{128}\beta^4 + \ldots \]  

\[ E^{(2)} = 3 + \frac{3}{2}\beta - \frac{3}{8}\beta^2 + \frac{3}{16}\beta^3 - \frac{15}{128}\beta^4 + \ldots \]  

Then, using the series for \( I = 1 \) up to \( E^{(1)}_{E_2} \) and \( I = 2 \) up to \( E^{(1)}_{E_1} \) as indicated by underlines in Eq. (31), we obtain the following results for \( \Pi_{[2]} \):

\[ \Pi_{[2],1} = 2 + \beta - \frac{1}{2}\sqrt{4 + 4\beta + 2\beta^2}, \]

\[ = 1 + \frac{1}{2}\beta - \frac{1}{8}\beta^2 + \frac{1}{16}\beta^3 - \frac{3}{128}\beta^4 + \ldots \]  

\[ \Pi_{[2],2} = 2 + \beta + \frac{1}{2}\sqrt{4 + 4\beta + 2\beta^2}, \]

\[ = 3 + \frac{3}{2}\beta + \frac{1}{8}\beta^2 - \frac{1}{16}\beta^3 + \frac{3}{128}\beta^4 + \ldots \]  

Here, we have underlined the terms that are correct in comparison with the exact results. Thus, we gain one order for \( E^{(1)} \) in comparison to the input data while there is no gain in \( E^{(2)} \).

The following theorem shows that the coefficients in \( P \)-type polynomials leading to approximants \( P_{[Q+1]} \) satisfy the equations for the polynomials leading to approximants \( P_{[Q]} \), and hence, these polynomials can be computed recursively.
THEOREM 1. Define

\[ P_N^{(Q)}(E) = E^N + \sum_{j=0}^{N-1} E^j \sum_{k=0}^{Q} a_k^{(j,Q)} \beta^k \]  

(33)

for all \( Q \) and given \( N \). The zeroes of the polynomial \( P_N^{(Q)} \) are the \( P \)-type approximants \( P_{[Q]} \), if for \( \beta \to 0 \)

\[ P_N^{(Q)} \left( \sum_{\ell=0}^{Q} E^{(I)}_\ell \beta^\ell \right) = O(\beta^{Q+1}) , \quad (I = 1, \ldots, N) \]  

(34)

holds. Assume that for \( I = 1, \ldots, N \)

\[ P_N^{(Q+1)} \left( \sum_{\ell=0}^{Q+1} E^{(I)}_\ell \beta^\ell \right) = O(\beta^{Q+2}) \]  

(35)

holds for \( \beta \to 0 \) whence the zeroes of this polynomial are the \( P \)-type approximants \( P_{[Q+1]} \). Define

\[ \tilde{P}_N^{(Q)}(E) = E^N + \sum_{j=0}^{N-1} E^j \sum_{k=0}^{Q} a_k^{(j,Q+1)} \beta^k . \]  

(36)

Then for \( \beta \to 0 \), the relations

\[ \tilde{P}_N^{(Q)} \left( \sum_{\ell=0}^{Q} E^{(I)}_\ell \beta^\ell \right) = O(\beta^{Q+1}) \]  

(37)

hold for \( I = 1, \ldots, N \), and thus, \( \tilde{P}_N^{(Q)} = P_N^{(Q)} \).

Proof. Put

\[ E^{(I,Q)}(\beta) = \sum_{\ell=0}^{Q} E^{(I)}_\ell \beta^\ell . \]  

(38)

Then direct calculation shows

\[ \tilde{P}_N^{(Q)}(E^{(I,Q)}(\beta)) = -\beta^{Q+1} [E^{(I,Q)}(\beta)]^{N-1} NE^{(I)}_{Q+1} \]

\[ -\beta^{Q+1} \sum_{j=0}^{N-1} j[E^{(I,Q)}(\beta)]^{j-1} E^{(I)}_{Q+1} \sum_{k=0}^{Q} a_k^{(j,Q+1)} \beta^k \]

\[ -\beta^{Q+1} \sum_{j=0}^{N-1} [E^{(I,Q)}(\beta)]^j a_{Q+1}^{(j,Q+1)} \]

\[ +O(\beta^{Q+2}) \]

\[ = O(\beta^{Q+1}) \]  

(39)
Table I. Quadratic P-type Approximants for the quartic AHO with $\beta = 1/100$

| $Q$ | $P_{[Q],1}$    | $P_{[Q],2}$    |
|-----|----------------|----------------|
| 2   | 1.007375       | 3.03646        |
| 3   | 1.0073736      | 3.03653        |
| 4   | 1.00737368     | 3.036525       |
| 5   | 1.00737371     | 3.0365254      |
| 6   | 1.0073736722   | 3.03652530     |
| 7   | 1.00737367206  | 3.036525306    |
| 8   | 1.00737367208  | 3.0365253043   |
| 9   | 1.007373672081 | 3.0365253045   |
| 10  | 1.0073736720815| 3.03652530451  |
| 11  | 1.00737367208137| 3.036525304514|
| 12  | 1.00737367208139| 3.0365253045131|
| 13  | 1.00737367208138| 3.0365253045134|
| 14  | 1.00737367208138| 3.03652530451334|
| 15  | 1.00737367208138| 3.03652530451335|
| $\infty$ | 1.00737367208138 | 3.03652530451335 |

Recursive algorithms are also known for certain algebraic approximants [21], and, more generally for the computation of Hermite-Padé polynomials [2, Sec. 8.5].

4. Numerical Tests

In the test cases, we always treat the quartic AHO with Hamiltonian as defined in Eq. (3) for small $\beta$ without any renormalization. The coefficients in all the perturbation series used below have been computed using RSPT up to order 20 in the wave functions, followed by Taylor expansion of the Rayleigh-Ritz expectation value with this wave function leading to the coefficients in the perturbation series for the energies up to order 41. The computations were done in MAPLE V™.

In Table I we consider quadratic P-type approximants ($N = S = 2$) for various values of $Q$. The calculation of approximants $P_{[Q],j}$ requires two $Q$-th order perturbation series for the two lowest eigenvalues. The results show that both eigenvalues are well approximated for $Q = 15$. 
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Table II. Π-type Approximants for the quartic AHO with $\beta = 1/100$

| $N$ | $\Pi_{[N],1}$   | $\Pi_{[N],2}$   |
|-----|-----------------|-----------------|
| 2   | 1.007371        | 3.0376          |
| 3   | 1.0073738       | 3.03650         |
| 4   | 1.007373667     | 3.0365266       |
| 5   | 1.0073736724    | 3.03652522      |
| 6   | 1.00737367206   | 3.036525310     |
| 7   | 1.00737367208   | 3.0365253040    |
| 8   | 1.0073736720812 | 3.03652530456   |
| 9   | 1.00737367208140| 3.036525304509  |
| 10  | 1.00737367208138| 3.0365253045138|
| $\infty$ | 1.00737367208138 | 3.03652530451335 |

Table III. $D$-type Approximants for the quartic AHO with $\beta = 2/10$

| $N$ | $D_{[N],1}$ | $D_{[N],2}$ |
|-----|-------------|-------------|
| 2   | 1.11        | 3.8         |
| 4   | 1.117       | 3.53        |
| 6   | 1.1181      | 3.534       |
| 8   | 1.11826     | 3.5377      |
| 10  | 1.11828     | 3.5386      |
| 12  | 1.118291    | 3.5389      |
| Exact | 1.118293    | 3.5390      |

The convergence of the approximants is somewhat faster for the lower eigenvalue.

In Table II, we consider Π-type approximants for various values of $N$. The calculation of approximants $\Pi_{[N],j}$ requires $N$ perturbation series with orders $N, N - 1, \ldots, 1$. Only the results for the two lowest eigenvalues are displayed for comparison reasons. The data show that Π-type approximants converge somewhat faster than $P$-type approximants in the example treated. The results show that both eigenvalues are well approximated for $N = 10$. The convergence of the approximants is somewhat faster for the lower eigenvalue.
For large $\beta$, both $\Pi$- and $P$-type approximants break down and start to produce complex approximants.

In Table III, we consider $D$-type approximants for various values of $N$ for a larger $\beta$. The calculation of approximants $D_{[N],j}$ requires $N$ perturbation series with orders $N, N-1, \ldots, 1$ (even $N$). Again, only the results for the two lowest eigenvalues are displayed for comparison reasons. The results indicate that this type of multiseries approximant can be useful for somewhat larger $\beta$. Comparison values are taken from Ref. [18].

In further studies it is planned to study these approximants also for renormalized perturbation series in order to see whether for these the range of applicability of the approximants is extended as is the case for several other methods.

5. Summary

- Effective characteristic polynomial approximants are special algebraic approximants.

- Polynomial-type multiseries approximants combine the information of several perturbation series and allow the summation of divergent series. They are different from Hermite-Padé approximants.

- Perturbation series for these multiseries approximants are less costly to calculate than for algebraic approximants (several short series vs. one long expansion).

- The simultaneous calculation of several eigenvalues is possible. Higher eigenvalues converge slower.

- The large number of variants of multiseries approximants should be explored further.

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