# Analytic-continuation approach to the resummation of divergent series in Rayleigh-Schrödinger perturbation theory

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The method of analytic continuation is applied to estimate eigenvalues of linear operators from finite order results of perturbation theory even in cases when the latter is divergent. Given a finite number of terms $E^{(k)}, k = 1, 2, \ldots M$ resulting from a Rayleigh-Schrödinger perturbation calculation, scaling these numbers by $\mu^k$ ($\mu$ being the perturbation parameter) we form the sum $E(\mu) = \sum_k \mu^k E^{(k)}$ for small $\mu$ values for which the finite series is convergent to a certain numerical accuracy. Extrapolating the function $E(\mu)$ to $\mu = 1$ yields an estimation of the exact solution of the problem. For divergent series, this procedure may serve as resummation tool provided the perturbation problem has a nonzero radius of convergence. As illustrations, we treat the anharmonic (quartic) oscillator and an example from the many-electron correlation problem.

## I. INTRODUCTION

Perturbative expansion of eigenvalues of linear operators [1] is a common tool in many areas of quantum physics when exact or numerically exact solutions are not feasible by other techniques. Experience in many-electron theory [2], for example, shows that Rayleigh-Schrödinger perturbation theory (RSPT) usually provides good approximations at low orders, but the series often proves to be divergent.

Although the *a priori* necessary and sufficient conditions for convergence in RSPT are unknown, the reasons for occurring divergence are well understood [1]. To recapitulate the essential points, consider a linear operator (e.g., a Hamiltonian $\hat{H}$) split as

$$\hat{H}(z) = \hat{H}^{(0)} + z\,\hat{W}. \tag{1}$$

We refer to $\hat{H}^{(0)}$ as the zero-order Hamiltonian and to $\hat{W}$ as the perturbation. The coupling parameter $z$ may or may not have a physical meaning; we use it here merely as a formal perturbation parameter. The case $z = 1$ refers to the situation of physical meaning. Considering the eigenvalue problem

$$\hat{H}(z)\,\Psi(z) = E(z)\,\Psi(z); \tag{2}$$

the eigenvalues $E(z)$ formally depend on the perturbation parameter, and RSPT provides us with its Taylor expansion

$$E(z) = \sum_{n=0}^{\infty} z^n E^{(n)} \tag{3}$$

with $E^{(n)}$ being the contribution to the eigenvalue at order $n$. Since we are interested in the physical value $E(z = 1)$, this Taylor series will be convergent if the complex function $E(z)$ is analytic inside and on the unit circle $|z| \leqslant 1$. Knowing the Hamiltonian at all complex values $z$, one may find its eigenvalues $E(z)$, and check whether any singularity spoils its analycity within the unit circle. Note that this analysis is more demanding than the original problem at $z = 1$, since $\hat{H}(z)$ is complex and not Hermitian for complex values of $z$. Nevertheless, such analyses can be found in literature (see, for example, Ref. [3]).

## II. THEORY

Let us suppose that the PT problem has been solved for the physical situation $z = 1$ up to a certain order $M$. This means one knows the contributions $E^{(n)}$ at $z = 1$ for $n \leqslant M$, hence the partial sum

$$E^{[M]} = \sum_{n=0}^{M} E^{(n)}$$

is available. For any value of $z$, one can easily [i.e., without resolving the eigenvalue problem of $\hat{H}(z)$] obtain the scaled values

$$E^{[M]}(z) = \sum_{n=0}^{M} z^n E^{(n)} \tag{4}$$

at practically no computational cost. The series above will converge fast (in the sense that the terms already around $M$ become negligible) for sufficiently small values of $|z|$, if the original series has a nonzero radius of convergence. The sum of the scaled series can thus be obtained within a given accuracy. Let us denote the largest value of $|z|$ for which the partial sum in Eq. (4) has manifestly converged (to a certain digit) by $|z_0|$. Then $|z_0|$ serves as a numerical estimation of the convergence radius of the expansion. Since for $|z| < |z_0|$ the convergence is ensured, $E(z)$ must be analytic there. The region $|z| < |z_0|$ can be called the trusted region.

We may try to use the $|z| < |z_0|$ domain of $E(z)$ and apply analytic continuation for $|z| > |z_0|$, in a fortunate case up to $z = 1$, along a contour which is free from any singularity of $E(z)$. For example, if no singularity appears on the real axis

in the interval $z_0 < z \leqslant 1$, $E(z)$ can be extrapolated for $z \in \mathbb{R}$ up to the point corresponding to the physical situation $z = 1$. In Sec. III, we shall show some actual examples for which this technique was working.

Among possible methods of analytic continuation, the simplest is to fit a polynomial $p(z)$ onto the converged points for $|z| < |z_0|$, and evaluate this polynomial at $z = 1$. The $p(1)$ value serves as en estimation to the exact eigenvalue of Eq. (1). This simple procedure may work quite well, although a polynomial form is fully adequate if function $E(z)$ is analytic everywhere on the complex plane, in which case RSPT is convergent for all $z$. Nevertheless, polynomial extrapolation along the real axis may be useful to sum up a divergent series, too, as demonstrated below.

A more sophisticated procedure is to find fitting functions which reflect the suspected singularity structure of $E(z)$. Such an idea was successfully used, in another context, by Jeziorski *et al.* in the field of intermolecular interactions treated perturbatively [4,5]. Here we test the applicability of the ratio of two polynomials (i.e., linear Padé approximants) [6], and quadratic Padé approximants. The relevant formulas can be given as a linear equation

$$q(z)E_{[NM]}(z) = p(z) \tag{5}$$

for linear Padé approximants yielding

$$E_{[NM]}(z) = \frac{p(z)}{q(z)}, \tag{6}$$

which may show a pole-type singularity, and as a second-order equation

$$r(z)E_{[NMR]}^2(z) + q(z)E_{[NMR]}(z) = p(z) \tag{7}$$

for the quadratic Padé approximants, having the solution

$$E_{[NMR]}(z) = \frac{-q(z) \pm \sqrt{q(z)^2 + 4r(z)p(z)}}{2r(z)} \tag{8}$$

exhibiting branch cuts potentially. In the above equations $p(z)$, $q(z)$, and $r(z)$ are polynomials of order $N, M, R$, respectively. We emphasize that, unlike in the conventional use of a Padé approximant, we do not solve Eqs. (5) and (7) up to a certain order, but we propose to fit the unknown coefficients in polynomials $p$, $q$, and $r$ to the scaled, convergent result in the trusted region of $E(z)$.

Several other techniques have been described to the resummation of divergent series. The simplest idea is to use linear [6] or quadratic [7] Padé approximants fitting them directly to the terms of the divergent series at $z = 1$ [8–10]. In many-electron theory, according to the experience gained in our laboratory [11], their predictions are rather uncertain. Standard mathematical resummation techniques like the Borel summation [12,13] cannot be used in this field, since in practice usually we do not know any formula for the series to be summed, just a certain (finite) number of terms.

### III. EXAMPLES

#### A. A trivial example

Suppose one is provided the series of numbers

$$1 - 2 + 4 - 8 + 16 - 32 \pm \dots,$$

which is clearly divergent. Scaling it with a real parameter (we use the notation $\mu$ instead of $z$ if the parameter is intentionally kept real) $0 < \mu < 1/2$ makes it convergent, since the series in question can be considered as the Taylor expansion of $1/(1 + 2x)$ for $x = 1$, and this expansion has a radius of convergence $1/2$. Choosing $\mu = 0.4$, e.g., yields the convergent series

$$f(0.4) = 1 - 0.8 + 0.64 - 0.512 + 0.410 - 0.327 \pm \dots$$
$$= 0.55\dot{5}.$$

Since the function has a pole at $x = -1/2$, there are no singularities in the interval [0,1]. Therefore, considering the scaled converged values, one may draw the function $f(\mu)$, and use a Padé approximant, as a function of $\mu$, to find an analytic form. The [0,1] Padé fits exactly, and gives the result of the resummation $1/(1 + 2) = 1/3$, at $\mu = 1$. We report less trivial examples below.

#### B. Anharmonic oscillator

Consider the Hamiltonian of the harmonic oscillator perturbed with a quartic term

$$\hat{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}\omega x^2 + \gamma x^4. \tag{9}$$

If the harmonic part is chosen as the zero-order Hamiltonian, so the perturbation is represented by the full quartic term $\gamma x^4$, RSPT is known to be divergent for all nonzero $\gamma$ values [14,15] due to a branching type singularity at the origin. In other words, the PT series as applied to the quartic anharmonic oscillators has a zero radius of convergence in this partitioning. This system seems therefore unsuitable for the resummation technique outlined in Sec. II which requires a nonzero radius of convergence. However, one can change the partition of the Hamiltonian, and apply the so-called Epstein-Nesbet (EN) partitioning [16,17], in which all diagonal matrix elements of $\gamma x^4$ are shifted to the zero order, resulting in zero first-order corrections. We have pointed out previously [18] that in the EN partitioning the RSPT has a finite radius of convergence; it is convergent, e.g., for $\gamma = 0.025$ but it is already divergent for $\gamma = 0.1$. The latter, divergent case is illustrated in Fig. 1.

We apply the scaling procedure as follows. In an interval $0 < \mu < |z_0|$ the PT in the EN partitioning is made convergent by scaling the original divergent energy contributions. In Table I we show the result for scaling values $\mu = 0.2, 0.4$, and 0.6, as examples. The numbers in the column $\mu = 1.0$ clearly indicate that the series is divergent (as illustrated also in Fig. 1). However, even for $\mu = 0.6$, the scaled series turns out to be nicely convergent. The last row of the table shows the sum of the contributions.

The scaled sums for a large number of values of $\mu$ are plotted in Fig. 2. The figure shows also the exact energy obtained by numerical solution of the Schrödinger equation, as well as the curve obtained by fitting a six-order polynomial to the scaled values. The fitted curve represents a very simple means of analytic continuation, and on the given scale of the figure (millihartrees) it matches the exact line at $\mu = 1$. The method described in Sec. II can therefore be used as a resummation technique for the divergent PT series of the anharmonic oscillator.
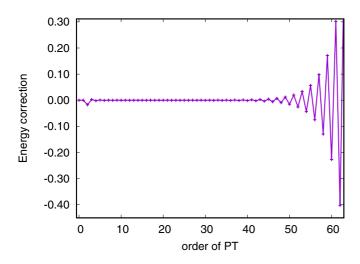
FIG. 1. Perturbational energy contributions for the quartic anharmonic oscillator in Epstein-Nesbet partitioning. The value of coupling constant is $\gamma = 0.1$. (Atomic units are used.)
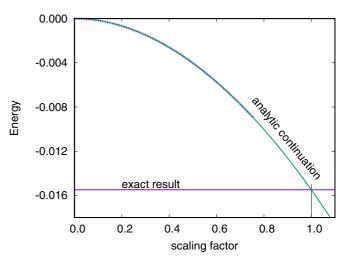


FIG. 2. Analytic continuation of the energy of the quartic anharmonic oscillator at coupling constant $\gamma = 0.1$. Scaled values are indicated by purple $+$ symbols.

To gain an insight into the accuracy of analytic continuation, we compare the results of a few fitting procedures in Table II. We start for a simple second-order polynomial, test a fourth-order one, and report the accuracy of a sixth-order polynomial (the latter was shown in Fig. 2). The table shows a gradual improvement when using fitting polynomials of order 2, 4, and 6, respectively.

Table II also shows extrapolated energies predicted by [2,2], [4,4], and [6,6] Padé approximants corresponding to Eq. (6). Although the [6,6] Padé approximant has greater flexibility, the predicted energy is almost the same as that of a sixth order polynomial, both showing an error of 1 microhartree. An

important difference from the polynomial case is that $[N,N]$ Padé approximants are less sensitive to $N$: already for $N = 2$ we obtain six-digit accuracy (the perfect match between $E[2,2]$ and the exact energy is accidental).

As to the performance of the quadratic Padé approximant of Eq. (8), as extrapolation tools, our experience is similar. Already $E[2,2,2]$ differs from the exact energy only by a few microhartrees, while $E[4,4,4]$ and $E[6,6,6]$ are practically exact.

It is also worth investigating how the predicted energies depend on the number of orders used. As it can be deduced from Table I, up to six-digit accuracy, four orders are necessary to consider for $\mu = 0.2$, and one needs ten orders for $\mu = 0.6$. As we checked, the series is definitely convergent up to $\mu = 0.7$, and at this point one needs 24 orders to achieve microhartree (i.e., six digits) accuracy. In Table III we collect a few numerical examples showing the relations among the size of the part of the trusted region used for fitting, the accuracy of the extrapolation, and the number of orders one has to know to carry out the procedure.

TABLE I. Perturbational energy contributions for the quartic anharmonic oscillator with the coupling constant value $\gamma = 0.1$ for a few selected values of the scaling parameter $\mu$. Scaling is done by $\mu^n$, $n$ being the order of perturbation.

| | Energy correction (a.u.) | | | |
| | Original | Scaled | | |
| Order $n$ | $\mu = 1.0$ | $\mu = 0.2$ | $\mu = 0.4$ | $\mu = 0.6$ |
|---|---|---|---|---|
| 0 | 0.0 | 0.000000 | 0.000000 | 0.000000 |
| 1 | 0.0 | 0.000000 | 0.000000 | 0.000000 |
| 2 | $-0.017660$ | $-0.000706$ | $-0.002826$ | $-0.006358$ |
| 3 | 0.003103 | 0.000025 | 0.000199 | 0.000670 |
| 4 | $-0.001817$ | $-0.000003$ | $-0.000047$ | $-0.000236$ |
| 5 | 0.000873 | 0.000000 | 0.000009 | 0.000068 |
| 6 | $-0.000567$ | $-0.000000$ | $-0.000002$ | $-0.000026$ |
| 7 | 0.000372 | 0.000000 | 0.000001 | 0.000010 |
| 8 | $-0.000273$ | $-0.000000$ | $-0.000000$ | $-0.000005$ |
| 9 | 0.000207 | 0.000000 | 0.000000 | 0.000002 |
| 10 | $-0.000167$ | $-0.000000$ | $-0.000000$ | $-0.000001$ |
| ... | | | | |
| 40 | $-0.001651$ | $-0.000000$ | $-0.000000$ | $-0.000000$ |
| ... | | | | |
| 50 | $-0.017227$ | $-0.000000$ | $-0.000000$ | $-0.000000$ |
| Sum | $\infty$ | $-0.000684$ | $-0.002666$ | $-0.005876$ |

TABLE II. Predicted values for the energy of quartic anharmonic oscillator with coupling constant $\gamma = 0.1$ as obtained from analytic continuation.

| Method of continuation | Energy (a.u.) |
|---|---|
| Polynomial of order 2 | $-0.016352$ |
| Polynomial of order 4 | $-0.015866$ |
| Polynomial of order 6 | $-0.015853$ |
| [2,2] linear Padé approximation | $-0.015854$ |
| [4,4] linear Padé approximation | $-0.015853$ |
| [6,6] linear Padé approximation | $-0.015855$ |
| [2,2,2] quadratic Padé approximation | $-0.015858$ |
| [4,4,4] quadratic Padé approximation | $-0.015853$ |
| [6,6,6] quadratic Padé approximation | $-0.015853$ |
| Exact solution | $-0.015854$ |

TABLE III. Dependence of the predicted energies as obtained by fitting [6,6,6] quadratic Padé approximants for the anharmonic oscillator from the size of the fitting region.

| Fitting region | $E_{[6,6,6]}$ | Number of orders used |
|---|---|---|
| [0 − 0.4] | 0.015868 | 6 |
| [0 − 0.5] | 0.015850 | 8 |
| [0 − 0.6] | 0.015851 | 10 |
| [0 − 0.7] | 0.015853 | 24 |
| Exact result | 0.015854 | $\infty$ |

### C. Correlation energy

Divergent perturbation series often emerge in many-electron theory when one tries to evaluate electron correlation energy perturbatively. Consider for example the dissociation problem of the water molecule in the Møller-Plesset partitioning [19], where the zero order is the Hartree-Fock, and electron correlation gives rise to the perturbation. Table IV presents the perturbation corrections of the energy at an elongated O—H distance (2.5 times the equilibrium bond length) in a basis set where each atomic valence orbital is described by three functions and a $d$ orbital on O is added (the so-called 6-311G* basis [20]). A few scaled series are also tabulated in columns 3–5 of the table at some selected values of $\mu$. Figure 3 shows the partial sums order by order at $\mu = 1$. While the original series is apparently divergent, scaling by small values of $\mu$ makes it fast converging (cf. Table IV) permitting one to find the sum of the series easily up to a certain number of digits (six in the tabulated examples). The chosen values of $\mu$ in Table IV are merely for illustration: Fig. 4 shows the $E(\mu)$ function plotted on a fine grid in the interval $0 < \mu < 0.7$. The upper limit of 0.7 was chosen to be confidently smaller than the observed convergence radius of the series. (To estimate the convergence radius, we used the method of quadratic Padé approximants as proposed by Goodson [7]. In the present case we have found a pair of points of singularity a little bit off the real axis predicting a convergence radius $\approx 0.9$, and a divergent PT series thereby [11].)

TABLE IV. Correlation energy of the water molecule with elongated OH bonds as obtained by many-body perturbation theory in the Møller-Plesset partitioning. Scaling is done by $\mu^n$, $n$ being the order of perturbation.

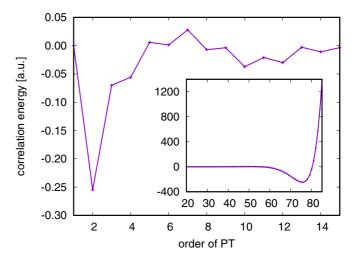| | Energy correction (a.u.) | | | |
|---|---|---|---|---|
| | Original | Scaled | | |
| Order | | | | |
| $n$ | $\mu = 1$ | $\mu = 0.3$ | $\mu = 0.2$ | $\mu = 0.1$ |
| 2 | −0.254895 | −0.022941 | −0.010196 | −0.002549 |
| 3 | −0.070076 | −0.001892 | −0.000561 | −0.000070 |
| 4 | −0.055826 | −0.000452 | −0.000089 | −0.000006 |
| 5 | 0.005759 | 0.000014 | 0.000002 | 0.000000 |
| 6 | 0.001211 | 0.000001 | 0.000000 | 0.000000 |
| 7 | 0.027852 | 0.000006 | 0.000000 | 0.000000 |
| 8 | −0.007082 | −0.000000 | −0.000000 | −0.000000 |
| 9 | −0.003692 | −0.000000 | −0.000000 | −0.000000 |
| 10 | −0.037333 | −0.000000 | −0.000000 | −0.000000 |
| $\infty$ | | −0.025264 | −0.010844 | −0.002625 |



FIG. 3. Convergence of the perturbation series of the correlation energy for the water molecule with elongated OH bond lengths in Møller-Plesset partitioning. The inset shows the divergence at large orders.

According to the proposed procedure, this function is continued analytically to the point $\mu = 1$. Figure 4 shows the result of one of the simplest methods of analytic continuation: least-squares fit of a polynomial of order 6 to the scaled values. The value of the curve at $\mu = 1$ can be considered as the result of the resummation of the divergent PT series.

In Table V we compare the resummed values obtained from simple polynomial fitting and using the ratio of two polynomials [linear Padé approximation, cf. Eq. (5)] to the result of exact diagonalization which is manageable in this case (the order of the matrix is 2 342 224). We were unsuccessful in fitting a quadratic Padé formula for this system. The data in Table V. indicate that, in spite of the strongly divergent nature of many-body Møller-Plesset perturbation theory in
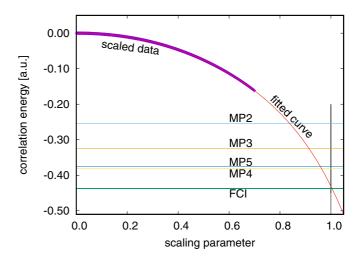


FIG. 4. Analytic continuation of the scaled sums of perturbative corrections for the correlation energy of the water molecule. The horizontal levels marked "MPn" indicate the energies of the PT series at order $n$. Dense purple dots indicate the scaled sums, continued by the red solid curve by polynomial fitting. The green horizontal line "FCI" indicates the correlation energy as obtained by exact diagonalization with the two core ($1s$) electrons kept frozen.

TABLE V. Correlation energy of the water molecule at 2.5 equilibrium distance predicted by analytic continuation.

| Method of continuation | Correlation energy (a.u.) |
| --- | --- |
| Polynomial of order [6] | − 0.43266 |
| [6,6] linear Padé approximation | − 0.43715 |
| Exact (full-CI) result | − 0.43725 |

this example, the analytic-continuation method provides an acceptable estimate, showing energy errors in the order of a millihartree or less.

## IV. CONCLUSION

The examples of the anharmonic oscillator and the correlation energy calculation by PT show that it may be possible to find a simple resummation procedure for a divergent PT series yielding physically relevant results. The technique proposed is to scale down the PT contributions with the relevant powers of the order parameter $\mu$ below the convergence radius of the series (i.e., to the trusted region), sum the series for several values of $\mu$, then continue analytically the function to the point $\mu = 1$.

Though evaluation of original PT contributions may be hard if the underlying problem is difficult, the extrapolation procedure we used here is practically costless: we merely manipulate with the numbers we have for the PT contributions.

Since the closed form of the summed values as a function of $\mu$ are usually not known, analytic continuation requires some numerical extrapolation procedure in practice. This raises several dilemmas. If polynomial extrapolation is applied, it is clearly useless to determine the coefficients of the polynomial (i.e., the derivatives of the function to be extrapolated) at $\mu = 0$, as it would simply recover the original (divergent) series. Resorting to very small values of $\mu$ inherits this problem, although it would ensure very fast convergence of the scaled series. On the other hand, using larger values of the order parameter makes it easier to extrapolate, but the slower

convergence for these values of $\mu$ may generate numerical uncertainties questioning the accuracy of the resummation. Here we decided to use the rather wide interval $\mu \in [0,0.7]$ for fitting the polynomial, which yielded the accuracy shown above.

Another dilemma is manifested in choosing the functional form of the function to fit. The polynomial is the simplest idea, but its order has to be carefully chosen to provide sufficient flexibility but avoid numerical uncertainties that may arise with high-order forms. As shown for the case of the anharmonic oscillator, a second-order polynomial can give only a meaningful estimate, while four- and six-order polynomials yield quite accurate results.

Somewhat more stable results were obtained if, instead of a simple polynomial, the ratio of two polynomials were applied as extrapolating functions. For the anharmonic oscillator, a [2,2] Padé approximant gives already a very nice result.

Since the singularities of functions $E(z)$ spoiling convergence of its perturbational expansions are often branchings, a virtually more sophisticated extrapolation function class is offered by quadratic Padé approximants Eqs. (5) and (6). For the example studied, we did not see much difference from linear Padé approximants; both were found to be quite accurate for the anharmonic oscillator. No reassuring results for quadratic Padé approximants have yet been obtained however for the water correlation energy.

Theoreticians are herewith invited to find extrapolation schemes better for this purpose, perhaps by finding more appropriate and flexible fitting functions. A robust solution of this question would add a more practical aspect to the ideas of conceptual importance reported above.

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