Performance of superconvergent perturbation theory

Ernst Joachim Weniger*
Institut für Physikalische und Theoretische Chemie, Universität Regensburg, D-93040 Regensburg, Federal Republic of Germany
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The performance of the so-called superconvergent perturbation theory [W. Scherer, Phys. Rev. Lett. **74**, 1495 (1995)] is investigated numerically in the case of the ground-state energy of a quartic anharmonic oscillator. It is shown that Scherer's superconvergent approximation, which is rational in the coupling constant β, gives in the case of small coupling constants somewhat better results than the strongly divergent but asymptotic Rayleigh-Schrödinger perturbation series if it is truncated at the same order in β. However, the transformation of this truncated perturbation series into Padé approximants or into another class of rational functions by means of the sequence transformation $\delta_k^{(n)}(\zeta,s_n)$ [E. J. Weniger, Comput. Phys. Rep. **10**, 189 (1989)] yields much more powerful rational approximants. Moreover, the performance of the superconvergent approximation can be improved considerably by Wynn's epsilon algorithm [P. Wynn, Math. Tables Aids Comput. **10**, 91 (1956)] or by $\delta_k^{(n)}(\zeta,s_n)$. Finally, it is shown that the other rational approximants provide much better approximations to higher order terms of the Rayleigh-Schrödinger perturbation series than Scherer's superconvergent approximation. [S1050-2947(97)02112-4]

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By means of some analogies with perturbation theories for classical Hamiltonian systems, Scherer [1,2] developed a new perturbation theory for Hamiltonians that can be expanded in a power series in the coupling constant β:

$$\hat{H}(\beta)=\sum_{n=0}^{\infty}\frac{\beta^n}{n!}\hat{H}_n . \tag{1}$$

As usual, it is assumed that the Hamiltonians $\hat{H}_n$ do not depend on β.

Ordinary Rayleigh-Schrödinger perturbation theory yields in the case of a discrete and nondegenerate spectrum a formal power series expansion in β for an energy eigenvalue $E(\beta)$ of the Hamiltonian (1):

$$E(\beta) \;=\; \sum_{n=0}^{\infty} c_n\beta^n . \tag{2}$$

In the case of Rayleigh-Schrödinger perturbation theory, the series coefficients c_n do not depend on β. Scherer's approach, which he called *superconvergent perturbation theory*, reproduces up to orders three in β the coefficients c_n of the Rayleigh-Schrödinger perturbation expansion (2). For orders four or higher in β, expansion coefficients result that depend explicitly on β.

In order to demonstrate the power of his approach, Scherer applied it in the case of the quartic anharmonic oscillator, which is defined by the following Hamiltonian:

$$\hat{H}(\beta) \;=\; \hat{p}^2+\hat{x}^2+\beta\hat{x}^4 \;,\; \beta\geqslant 0 . \tag{3}$$

Scherer [1] considered only approximations to the ground state energy that are of fourth order in β. In the case of the Rayleigh-Schrödinger perturbation theory this leads to following truncated perturbation series:

$$E_{\mathrm{RS}}^{(4)}(\beta)=1+\frac{3}{4}\beta-\frac{21}{16}\beta^2+\frac{333}{64}\beta^3-\frac{30\,885}{1024}\beta^4. \tag{4}$$

The series coefficients, which are rational numbers, can be computed by solving a system of nonlinear difference equations (compare, for instance, the appendix of Ref. [3]).

By including exactly all contributions up to order four in β, Scherer [1] obtained the following superconvergent approximation to the ground-state energy of the quartic anharmonic oscillator:

$$E_{\mathrm{su}}^{(4)}(\beta)=1+\frac{3}{4}\beta-\frac{21}{16}\beta^2+\frac{333}{64}\beta^3-\frac{3(131\,7760+129\,354\,72\beta+364\,333\,68\beta^2+251\,833\,05\beta^3)}{2048(4+9\beta)(4+15\beta)(4+21\beta)}\beta^4. \tag{5}$$

If we compare the approximants (4) and (5), which are both of order $O(\beta^5)$ as $\beta\to 0$, we see that Scherer's superconvergent perturbation theory essentially introduces a coefficient of β^4 that is rational in β. Since rational functions normally give much better results than truncated power series expansions, the superconvergent approximation (5) should yield more accurate approximations to the ground state energy of the anharmonic oscillator than the truncated Rayleigh-Schrödinger perturbation series (4). This is probably the reason why Scherer, who did not present any numerical results, called his perturbation theory *superconvergent*.

Nevertheless, the approximants (4) and (5) are not suited

*Electronic address:
joachim.weniger@chemie.uni-regensburg.de

to demonstrate the superiority of superconvergent over ordinary Rayleigh-Schrödinger perturbation theory. Ever since the seminal work of Bender and Wu [4], the Rayleigh-Schrödinger perturbation series for the ground-state energy $E(\beta)$ of the quartic anharmonic oscillator has been the model example of a perturbation series that is only asymptotic as $\beta\to 0$ and that diverges quite strongly for every $\beta\neq 0$ [5]. As is well known, the accuracy that can be obtained by truncating a divergent asymptotic power series at the minimal term depends on the magnitude of the argument. Thus, reasonably accurate approximations to $E(\beta)$ can be obtained by truncating the divergent perturbation series if β is sufficiently small. If, however, β is not small, accurate approximations can only be obtained if the divergent perturbation series is used as the starting point of a summation process. Thus, Scherer's superconvergent approximation (5), which because of its rational nature can also be considered to be a summation method, should not be compared with the truncated Rayleigh-Schrödinger perturbation series (4) but with other rational approximants that can be constructed from it.

In applied mathematics and in theoretical physics, Padé approximants [6] have become the standard tool to sum divergent power series. For example, the computer algebra system MAPLE—which will be used quite extensively in this Brief Report—contains explicit commands to convert the partial sums of a power series to Padé approximants. Otherwise, Padé approximants can be computed conveniently with the help of Wynn's celebrated recursive epsilon algorithm [7]:

$$\epsilon_{-1}^{(n)}=0,\quad \epsilon_{0}^{(n)}=s_n, \tag{6a}$$

$$\epsilon_{k+1}^{(n)}=\epsilon_{k-1}^{(n+1)}+1/[\epsilon_{k}^{(n+1)}-\epsilon_{k}^{(n)}]. \tag{6b}$$

If the input data s_n for the epsilon algorithm are the partial sums $f_n(z)=\Sigma_{\nu=0}^{n}\gamma_\nu z^\nu$ of a formal power series for some function $f(z)$, the elements $\epsilon_{2k}^{(n)}$ with *even* subscripts are Padé approximants according to

$$\epsilon_{2k}^{(n)}=[n+k/k]_f(z). \tag{7}$$

The elements $\epsilon_{2k+1}^{(n)}$ with *odd* subscripts are only auxiliary quantities that diverge if the whole process converges.

The truncated Rayleigh-Schrödinger perturbation series (4) can be transformed into the following [2/2] Padé approximant:

$$\epsilon_{\rm RS}(\beta)=2\frac{1984+15\,862\beta+19\,567\beta^2}{3968+28\,748\beta+22\,781\beta^2}. \tag{8}$$

Padé approximants are not necessarily the most efficient rational approximants for the summation of strongly divergent perturbation series. A different class of rational approximants can be obtained with the help of the following sequence transformation [Eq. (8.4-4) of Ref. [8]], which is applied to the partial sums $s_n=\Sigma_{\nu=0}^{n}a_\nu$ of an infinite series:

$$\delta_k^{(n)}(\zeta,s_n)=\frac{\Sigma_{j=0}^{k}(-1)^j\binom{k}{j}[(\zeta+n+j)_{k-1}/(\zeta+n+k)_{k-1}]\ s_{n+j}/a_{n+j+1}}{\Sigma_{j=0}^{k}(-1)^j\binom{k}{j}[(\zeta+n+j)_{k-1}/(\zeta+n+k)_{k-1}]\ 1/a_{n+j+1}}. \tag{9}$$

Here, ζ is a parameter that has to be positive. The most obvious choice would be $\zeta=1$.

It was shown in several articles that the sequence transformation $\delta_k^{(n)}(\zeta,s_n)$, which can also be computed recursively [8], is able to sum effectively many strongly divergent quantum-mechanical perturbation expansions [3,9–14] and divergent asymptotic series for special functions [8,9,15,16]. Further details on $\delta_k^{(n)}(\zeta,s_n)$ and on related transformations can be found in Refs. [3,8,11,17,18], in Sec. 2.7 of the book by Brezinski and Redivo Zaglia [19], or in an article by Roy, Bhattacharya, and Bhowmick [20].

Application of the sequence transformation (9) with $k=3$, $n=0$, and $\zeta=1$ to the truncated Rayleigh-Schrödinger perturbation series (4) yields the following rational function:

$$\delta_{\rm RS}(\beta)=4\frac{33\,152+370\,776\beta+901\,569\beta^2+366\,040\beta^3}{132\,608+138\,3648\beta+274\,2588\beta^2+533\,281\beta^3}. \tag{10}$$

Wynn's epsilon algorithm, Eq. (6), is normally used for the transformation of the partial sums of a formal power series into Padé approximants according to Eq. (7). However, it can also be applied to other types of slowly convergent or divergent sequences such as, for instance, the partial sums of Scherer's superconvergent approximation (5). This yields the following expression, which is also rational in β but not a Padé approximant:

$$\epsilon_{\rm su}(\beta)=2[A_\epsilon(\beta)/B_\epsilon(\beta)], \tag{11a}$$

$$A_\epsilon(\beta)=550\,018\,35\beta^5-426\,119\,94\beta^4-786\,763\,20\beta^3-317\,094\,08\beta^2-488\,7296\beta-253\,952, \tag{11b}$$

$$B_\epsilon(\beta)=103\,157\,145\beta^5-333\,375\,48\beta^4-124\,258\,992\beta^3-570\,401\,92\beta^2-939\,3664\beta-507\,904. \tag{11c}$$

Similarly, the sequence transformation $\delta_k^{(n)}(\zeta,s_n)$, Eq. (9), is not restricted to power series and can also be applied to the

TABLE I. Performance of the truncated Rayleigh-Schrödinger perturbation series for the ground-state energy of the quartic anharmonic oscillator, of Scherer's superconvergent approximation, and of the other rational approximations for different values of the coupling constant β.

β	$E_{RS}^{(4)}(\beta)$	$E_{su}^{(4)}$	$\epsilon_{RS}(\beta)$	$\delta_{RS}(\beta)$	$\epsilon_{su}(\beta)$	$\delta_{su}(\beta)$	Exact
0.010	1.007 3737	1.007 3737	1.007 3737	1.007 3737	1.007 3737	1.007 3737	1.007 3737
0.025	1.017 9992	1.017 9996	1.018 0008	1.018 0010	1.018 0011	1.018 0012	1.018 0010
0.050	1.034 6807	1.034 6926	1.034 7254	1.034 7288	1.034 7319	1.034 7346	1.034 7297
0.075	1.050 1080	1.050 1936	1.050 4116	1.050 4304	1.050 4479	1.050 4616	1.050 4340
0.100	1.064 0620	1.064 4042	1.065 2179	1.065 2769	1.065 3347	1.065 3737	1.065 2855
0.150	1.085 2602	1.087 6170	1.092 6150	1.092 8822	1.093 1711	1.093 3148	1.092 9050
0.200	1.090 8672	1.099 9570	1.117 5406	1.118 2589	1.119 1183	1.119 4180	1.118 2926
0.250	1.068 9507	1.094 5322	1.140 3997	1.141 8723	1.143 8188	1.144 2480	1.141 9018
0.300	1.003 0542	1.062 1277	1.161 4847	1.164 0461	1.167 7818	1.168 1854	1.164 0472
0.350	0.872 1973	0.991 3248	1.181 0200	1.185 0157	1.191 4383	1.191 4882	1.184 9585
0.400	0.650 8750	0.868 5770	1.199 1863	1.204 9580	1.215 1754	1.214 3328	1.204 8103
0.450	0.309 0586	0.678 2601	1.216 1324	1.224 0098	1.239 3619	1.236 8392	1.223 7391
0.500	−0.187 8052	0.402 7055	1.231 9837	1.242 2784	1.264 3692	1.259 0882	1.241 8541

partial sums of Scherer's superconvergent approximation (5). Thus, the application of $\delta_k^{(n)}(\zeta,s_n)$ with $k=3$, $n=0$, and $\zeta=1$ yields

$$\delta_{su}(\beta)=4[A_\delta(\beta)/B_\delta(\beta)], \qquad (12a)$$

$$A_\delta(\beta)=212\,172\,80+475\,991\,040\beta+377\,654\,9376\beta^2 +135\,545\,497\,12\beta^3+230\,043\,300\,00\beta^4 +181\,592\,550\,27\beta^5+725\,743\,5570\beta^6, \qquad (12b)$$

$$B_\delta(\beta)=848\,691\,20+184\,031\,2320\beta+138\,373\,539\,84\beta^2 +458\,140\,086\,40\beta^3+688\,027\,143\,84\beta^4 +429\,804\,045\,72\beta^5+652\,247\,5995\beta^6. \qquad (12c)$$

In Table I, the truncated Rayleigh-Schrödinger perturbation series $E_{RS}^{(4)}(\beta)$, Eq. (4), is compared with Scherer's rational approximant $E_{su}^{(4)}$, Eq. (5), with the rational approximants $\epsilon_{RS}(\beta)$, Eq. (8), and $\delta_{RS}(\beta)$, Eq. (10), which were obtained by transforming $E_{RS}^{(4)}(\beta)$, and with the rational approximants $\epsilon_{su}(\beta)$, Eq. (11), and $\delta_{su}(\beta)$, Eq. (12), which were obtained by transforming $E_{su}^{(4)}$. The results in Table I show that $E_{su}^{(4)}$ gives for $\beta\leqslant 0.2$ only marginally better results than $E_{RS}^{(4)}(\beta)$. For $\beta>0.3$, both $E_{RS}^{(4)}(\beta)$ and $E_{su}^{(4)}$ produce nonsensical results. Much better results—in particular for larger values of β—are obtained by the [2/2] Padé approximant $\epsilon_{RS}(\beta)$ and even more so by the rational approximant $\delta_{RS}(\beta)$, which clearly gives best results (compare also Tables IV–VI of Ref. [3]). Moreover, $\epsilon_{su}(\beta)$ and $\delta_{su}(\beta)$ give clearly better results than $E_{su}^{(4)}$, from which they were derived. However, they are not as efficient as $\epsilon_{RS}(\beta)$ or $\delta_{RS}(\beta)$, which were derived from $E_{RS}^{(4)}(\beta)$. The results in Table I show that all other rational approximants give better results than Scherer's superconvergent approximation $E_{su}^{(4)}$.

The "exact" results in Table I were obtained by summing the renormalized perturbation series for the ground-state energy of the quartic anharmonic oscillator with the help of the sequence transformation $\delta_k^{(n)}(\zeta,s_n)$ as described in Ref. [3].

There is also another possibility of analyzing the power of a rational approximant. As is well known [6] a Padé approximant $[\ell/m]_f(z)=p_\ell(z)/q_m(z)$ to a function $f(z)=\sum_{\nu=0}^{\infty}\gamma_\nu z^\nu$ is constructed in such a way that its Taylor expansion coincides with the formal power series as far as possible, i.e.,

$$f(z)-p_\ell(z)/q_m(z)=O(z^{\ell+m+1}), \quad z\to 0. \qquad (13)$$

This asymptotic estimate implies that a Taylor expansion around $z=0$ reproduces all terms of the power series, which were used for the construction of the Padé approximant.

This *order-by-accuracy* principle holds also in the case of many other rational approximants. If $\delta_k^{(n)}(\zeta,s_n)$, Eq. (9), is applied to the partial sums $f_n(z)=\sum_{j=0}^{n}\gamma_j z^j$, a rational function $\delta_k^{(n)}(\zeta,f_n(z))$ with numerator and denominator polynomials of degrees $k+n$ and k results [Eq. (4.27) of Ref. [3]]. If the coefficients γ_n of the power series for $f(z)$ are all nonzero, the asymptotic error estimate [Eq. (4.29) of Ref. [3]]

$$f(z)-\delta_k^{(n)}(\zeta,f_n(z))=O(z^{k+n+2}), \quad z\to 0 \qquad (14)$$

holds, which shows that all terms that were used for the construction of $\delta_k^{(n)}(\zeta,f_n(z))$ are reproduced exactly by a Taylor expansion around $z=0$.

No general statement can be made about the behavior of the higher terms of the Taylor expansion of either the Padé approximant $[\ell/m]_f(z)$ or of the rational function $\delta_k^{(n)}(\zeta,f_n(z))$, which do not reproduce exactly the terms of the power series for $f(z)$. If, however, $[\ell/m]_f(z)$ and $\delta_k^{(n)}(\zeta,f_n(z))$ converge to $f(z)$ more rapidly than the partial sums $f_n(z)=\sum_{j=0}^{n}\gamma_j z^j$, then also the higher terms of the Taylor expansions of these rational functions should ultimately converge to the corresponding terms of the power series for $f(z)$. Consequently, at least the leading terms of the Taylor expansions of the differences $p_\ell(z)/q_m(z)-f_{\ell+m}(z)$ and $\delta_k^{(n)}(\zeta,f_n(z))-f_{k+n+1}(z)$ should provide *approximations* to the corresponding terms of the power series for $f(z)$.

It seems that this idea was first formulated and used by Gilewicz [21] in the context of Padé approximants. Later, this prediction property of Padé approximants was used by Samuel, Ellis, and Karliner [22] in connection with perturbative QCD calculations. Analogous prediction properties of sequence transformations were discussed by Sidi and Levin [23] and by Brezinski [24].

TABLE II. Approximations to the coefficients c_n with $n=5,6,7$ of the perturbation series for the ground-state energy of the quartic anharmonic oscillator obtained by performing Taylor expansions of Scherer's superconvergent approximation and of the other rational approximations around $\beta=0$.

n	Exact	$E_{su}^{(4)}$	$\epsilon_{RS}(\beta)$	$\delta_{RS}(\beta)$	$\epsilon_{su}(\beta)$	$\delta_{su}(\beta)$
5	223.8	43.2	188.6	212.4	231.9	255.6
6	−1999.5	−115.8	−1193.6	−1613.1	−1936.0	−2484.6
7	20 777.1	335.6	7564.2	12 559.8	16 534.4	24 869.7

Because of Eqs. (13) and (14), respectively, Taylor expansions of the rational functions $\epsilon_{RS}(\beta)$, Eq. (8), and $\delta_{RS}(\beta)$, Eq. (10), around $\beta=0$ produce expressions of the following kind:

$$\epsilon_{RS}(\beta)=E_{RS}^{(4)}(\beta)+e_5\beta^5+e_6\beta^6+e_7\beta^7+\cdots, \tag{15}$$

$$\delta_{RS}(\beta)=E_{RS}^{(4)}(\beta)+d_5\beta^5+d_6\beta^6+d_7\beta^7+\cdots. \tag{16}$$

As mentioned above, there is no reason to assume that the coefficients e_ν and d_ν with $\nu\geqslant 5$ would reproduce the corresponding coefficients c_ν of the Rayleigh-Schrödinger perturbation series exactly. Nevertheless, it should be interesting to see how well the exact coefficients

$$c_5=916\,731/4096, \tag{17}$$

$$c_6=-\,655\,184\,01/32\,768, \tag{18}$$

$$c_7=272\,329\,4673/131\,072 \tag{19}$$

are approximated by the coefficients e_5, e_6, e_7 and d_5, d_6, d_7 in Eqs. (15) and (16), respectively.

Table II lists the approximations to the exact perturbation series coefficients c_n with $n=5,6,7$, which are obtained by performing Taylor expansions around $\beta=0$ of Scherer's rational approximant $E_{su}^{(4)}$, Eq. (5), of the rational approximants $\epsilon_{RS}(\beta)$, Eq. (8), and $\delta_{RS}(\beta)$, Eq. (10), which were obtained by transforming $E_{RS}^{(4)}(\beta)$, and of the rational approximants $\epsilon_{su}(\beta)$, Eq. (11), and $\delta_{su}(\beta)$, Eq. (12), which were obtained by transforming $E_{su}^{(4)}$. The approximations to the coefficients were obtained by applying the MAPLE command Taylor to the symbolic expressions for the rational functions. The resulting coefficients, which are exact rational numbers, were then converted to floating-point numbers. In the case of $\epsilon_{su}(\beta)$ and $\delta_{su}(\beta)$ it is not known how many terms of the perturbation series would be reproduced exactly. It turned out that all rational approximants considered here reproduce exactly the truncated perturbation series $E_{RS}^{(4)}(\beta)$, Eq. (4).

The results in Table II show that Scherer's rational approximant $E_{su}^{(4)}$ produces only relatively poor approximations to the perturbation coefficients c_5, c_6, and c_7. The other rational approximants produce much better approximations upon Taylor expansion. In view of the simplicity of these rational approximants, the predicted values of the perturbation coefficients are actually remarkably accurate.

Of course, it is not yet possible to make a definite assessment of the usefulness of Scherer's superconvergent perturbation theory. First it would be necessary to know higher-order terms of Scherer's perturbation expansion for the ground-state energy of the quartic anharmonic oscillator. Moreover, it would be interesting to see how Scherer's approach performs in the case of other systems. Nevertheless, on the basis of the available data there is no evidence that the attribute *superconvergent* would be justified.

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