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Renormalized Rayleigh–Schrödinger perturbation theory*

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One method which has been used in the literature to determine the eigenvalues $F_k^{(0)}$ of a hamiltonian operator $\mathcal{H}=\mathcal{T}+\mathcal{W}$ ($\mathcal{T}=$kinetic energy operator) is to apply an approximation scheme (e.g. variational method) to the operator $\mathcal{H}_R(\beta)=\mathcal{T}+\mathcal{V}+\beta(\mathcal{W}-\mathcal{V})$ with eigenvalues $G_k(\beta)$, where the eigenvalue problem associated with $\mathcal{H}^{(0)}=\mathcal{T}+\mathcal{V}$ is solvable. Specifically, $F_k^{(0)}=G_k(1)$. We investigate the method from a perturbation theoretic viewpoint. There is a "renormalization map" $R:\beta\to\lambda$, $\beta\in[0,1]$, $\lambda\in[0,\infty)$, which relates the $G(\beta)$ to the eigenvalues $E(\lambda)$ of $\mathcal{H}(\lambda)=\mathcal{T}+\mathcal{V}+\lambda\mathcal{W}$. This, in turn, implies a linear relationship between the Rayleigh-Schrödinger β-series coefficients $G^{(n)}$ and the λ-series coefficients $E^{(n)}$ of the form $\boldsymbol{G}=\boldsymbol{C}\boldsymbol{E}$, where $\boldsymbol{C}$ is an infinite lower-triangular matrix. The "renormalized" β-series, $0\le\beta\le 1$, is useful in the accurate computation of $F^{(0)}$ as well as the eigenvalues $E(\lambda)$, $0\le\lambda<\infty$. In standard cases, the β-series is Borel summable to $G(\beta)$. Applications are made to anharmonic oscillators and hydrogen atoms in radial fields.

Key words: Perturbation theory — Summability

1. Introduction

Some years ago, Bell et al. [1] calculated eigenvalues of N-dimensional quartic oscillators given by the hamiltonians (in atomic units, rescaled here),

$$\mathcal{H}=p^2+r^4, \tag{1.1}$$

using the Rayleigh–Ritz variational method. They performed these calculations in the complete basis of (discrete) eigenfunctions of the N-dimensional oscillator

$$\mathcal{H}_{HO}=p^2+r^2 \tag{1.2}$$

by constructing the hamiltonian

$$\mathcal{H}_R(\beta)=\mathcal{H}_{HO}+\beta(r^4-r^2),\qquad 0\le\beta\le 1. \tag{1.3}$$

* Dedicated to Professor J. Koutecký on the occasion of his 65th birthday

The case $\beta = 1$ clearly corresponds to (1.1), whereas $\beta = 0$ corresponds to the "unperturbed" hamiltonian in (1.2). An intermediate value of β corresponds to a mixing of harmonic and quartic terms. From a theoretical chemical point of view, this mixing could conceivably model a realistic molecular vibration potential. In this report we wish to examine (albeit nonrigorously) the technique exemplified in Eq. (1.3) from the viewpoint of perturbation theory, especially in light of some basic knowledge about Rayleigh-Schrödinger (RS) expansions, their large order behavior, and their summability. (For a review of the progress of large order perturbation theory (LOPT) and its applications in theoretical physics and quantum chemistry, we refer the reader to [2] which contains the contributions to the 1981 Sanibel Workshop on LOPT.)

To illustrate, let us remark upon the above example. The case $\beta = 1$ in Eq. (3) corresponds to an "infinite-field limit" of perturbation theory. Consider the following anharmonic oscillator hamiltonian

$$\mathscr{H}(\lambda) = p^2 + r^2 + \lambda r^4, \qquad \lambda > 0. \tag{1.4}$$

Travelling the route of RSPT, we construct the series expansions

$$E(\lambda) = \sum_{n=0}^{\infty} E^{(n)} \lambda^n \tag{1.5}$$

for the various states. Equation (1.4) represents a *singular* perturbation [3], (i.e. r^4 grows faster than r^2) and the series in (1.5) is divergent. If we perform the Symanzik scaling transformation [4] $r \to \alpha r$, $\alpha \in \boldsymbol{R}$ (the transformation is unitary), multiply the Schrödinger equation associated with (1.4) by α^2, then set $\alpha = \lambda^{-1/6}$, we obtain a new eigenvalue problem

$$\mathscr{H}_\infty(\mu) = F(\mu), \tag{1.6}$$

where

$$\mathscr{H}_\infty(\mu) = p^2 + r^4 + \mu r^2 \tag{1.7}$$

and

$$F(\lambda^{-2/3}) = \lambda^{-1/3} E(\lambda). \tag{1.8}$$

Equation (1.7) represents a *regular* perturbation in the parameter $\mu = \lambda^{-2/3}$ (i.e. r^2 is bounded relative to r^4), so $F(\mu)$ has an expansion

$$F(\mu) = \sum_{n=0}^{\infty} F^{(n)} \mu^n, \tag{1.9}$$

which converges for $\mu < R$, where $0 < R < \infty$. Note that $F^{(0)}$ represents the appropriate eigenvalue of the hamiltonian in (1.1), which is obtained in the limit $\lambda \to \infty$, hence the term "infinite field limit". Moreover, Eq. (1.8) gives the large-λ behavior of the eigenvalues $E(\lambda)$ of (1.4):

$$E(\lambda) \approx \lambda^{1/3} \sum_{n=0}^{\infty} F^{(n)} \lambda^{-2n/3}, \qquad \lambda \to \infty. \tag{1.10}$$

In practice, however, it is generally difficult to compute the coefficients $F^{(n)}$.

One of the goals of LOPT has been to calculate the infinite-field eigenvalues $F^{(0)}$ from the "low-field" RS perturbation series [5]. It has been shown [6] that continued fraction representations of RS perturbation can be used in this regard. However, from a RSPT viewpoint, a technique like Eq. (1.3) yields such infinite field behavior with lesser effort. The basic idea of this approach is as follows. Start with a standard Schrödinger eigenvalue problem

$$[\mathscr{H}^{(0)}+\lambda \mathscr{W}]\psi(\lambda)=E(\lambda)\psi(\lambda), \tag{1.11}$$

where $\mathscr{W}$ is generally a singular perturbation and the solvable "unperturbed" eigenvalue problem is given by

$$\mathscr{H}^{(0)}\psi_k^{(0)}=(\mathscr{T}+\mathscr{V})\psi_k^{(0)}=E_k^{(0)}\psi_k^{(0)}. \tag{1.12}$$

Here, $\mathscr{T}$ is the kinetic energy operator, $\mathscr{V}$ a potential energy operator and the index $k=(k_1,\ldots,k_n)$ enumerates quantum states completely. Note that here we are working with the relatively simple problem of determining perturbations of discrete (bound) states. Associated with Eq. (1.11) are the standard RS expansions

$$E_k(\lambda)=\sum_{n=0}^{\infty} E_k^{(n)}\lambda^n. \tag{1.13}$$

We now wish to calculate the eigenvalues of the (infinite field) eigenvalue problem

$$\mathscr{H}'\psi'_{k'}=(\mathscr{T}+\mathscr{W})\psi'_{k'}=F_{k'}\psi'_{k'}, \tag{1.14}$$

this time, if possible, from RSPT. Here we are assuming that the state k' is obtained from the state k in (1.12) in a continuous fashion. Again, this problem may usually be derived from Eq. (1.11) by an appropriate scaling transformation:

$$[\mathscr{T}+\mathscr{W}+\lambda^{-a}\mathscr{V}]\psi(\lambda)=\lambda^{-b}E(\lambda)\psi(\lambda), \qquad a,b>0, \tag{1.15}$$

which implies that

$$E(\lambda)\approx F^{(0)}\lambda^{b} \quad \text{as } \lambda\to\infty. \tag{1.16}$$

In the spirit of Eq. (1.3), we define the following "renormalized" hamiltonian with eigenvalues $G(\beta)$,

$$\mathscr{H}_R(\beta)=\mathscr{T}+\mathscr{V}+\beta(\mathscr{W}-\mathscr{V})=G(\beta). \tag{1.17}$$

It follows that

$$G_k^{(0)}=G_k(0)=E_k^{(0)} \tag{1.18}$$

and

$$G_k(1)=F_{k'}^{(0)}. \tag{1.19}$$

We adopt a perturbative method of evaluating $G_k(1)$, i.e. construct the RS expansion for Eq. (1.17),

$$G(\beta)=\sum_{n=0}^{\infty} G^{(n)}\beta^n. \tag{1.20}$$

Since Eq. (1.17) still represents a singular perturbation problem, the series in (1.20) may be divergent. Nevertheless, in well-behaved cases, like those considered below, the series may still be summable.

We shall refer to the β-series in (1.20) as the "renormalized" perturbation series corresponding to the RS series in (1.13). There is a justification for this nomenclature, since, as will be seen for the examples studied, the coefficients $G^{(n)}$ and $E^{(n)}$ (corresponding to the same state) are related by a linear transformation of the following form

$$G^{(n)} = \sum_{m=0}^{n} c_{nm} E^{(m)}. \tag{1.21}$$

In other words, if we let $\boldsymbol{E} = (E^{(1)}, E^{(2)}, \ldots)^t$ and $\boldsymbol{G} = (G^{(1)}, G^{(2)}, \ldots)^t$ then

$$\boldsymbol{G} = \boldsymbol{C}\boldsymbol{E}, \tag{1.22}$$

where $\boldsymbol{C}$ is an infinite lower-triangular transformation matrix whose truncations are invertible. Moreover, a problem defined over the infinite range of coupling constant values $0 \le \lambda < \infty$ has been replaced by one defined over the finite interval $0 \le \beta \le 1$. A similar renormalization occurs in the Wick-ordering of simple quantum field theories, like the ϕ^4 model [7, 8]. More will be said on this relation below.

The approach outlined above will be applied to two major types of hamiltonians which have served as excellent testing grounds for perturbation methods:

(a) one-dimensional anharmonic oscillators (AHO), given by the hamiltonians

$$\mathcal{H}^m(\lambda) = -\frac{d^2}{dx^2} + x^2 + \lambda x^{2m} = E_K^m(\lambda), \qquad m = 2, 3, 4, \ldots \tag{1.23}$$

with unperturbed eigenvalues $E_K^m(0) = E_K^{(0),m} = 2K+1$, $K = 0, 1, 2, \ldots,$

(b) three (space)-dimensional hydrogen atoms in radial fields

$$\mathcal{H}^p(\lambda) = -\tfrac{1}{2}\nabla^2 - \frac{1}{r} + \lambda r^p = E_{NLM}^p(\lambda), \qquad p = 1, 2, 3, \ldots, \tag{1.24}$$

with unperturbed eigenvalues $E_{NLM}^p(0) = E_{NLM}^{(0),p} = -(2N^2)^{-1}$.

The extension of these hamiltonians to arbitrary spatial dimensions is straightforward. In order to minimize any notational complications, λ will represent the formal perturbation parameter in both problems. The renormalized parameter will be represented by β.

It is also noteworthy to mention that there is no loss of generality in the choice of anharmonic oscillator hamiltonians in Eq. (1.23). Any oscillator problem of the form

$$\mathcal{H}(\lambda) = -a_1 \frac{d^2}{dx^2} + a_2 x^2 + a_3 \lambda x^{2m} = F(\lambda) \tag{1.25}$$

may be easily transformed into (1.23) by the scaling transformation $x \to \tau^{1/2}x$ so that

$$F(\lambda)=\tau^{-1}E\left(\frac{a_3}{a_1}\tau^{m+1}\lambda\right), \qquad \tau=\left(\frac{a_1}{a_2}\right)^{1/2}. \tag{1.26}$$

The parameter a_2 is important in quantum field theories and a_1 in quark confinement studies [9] since they contain the mass term. In theoretical spectroscopy, the parameters a_2 and a_3 (and λ) can adjust the mixing of harmonic and anharmonic terms in intramolecular vibrational potentials.

The layout of the rest of this paper is as follows. Section 2 outlines the main aspects of RSPT, summability methods and hydrogenic perturbation theory which form the basis of this study. In Sect. 3, we look at the anharmonic oscillators of (1.23) and analyze the rescaling of the quartic AHO, $m=2$. In Sect. 4, the hydrogenic problems of Eq. (1.24) are considered, with a specific application to the "charmonium" case $p=1$. In Sect. 5, we use the renormalized perturbation series to accurately calculate eigenvalues $E(\lambda)$ for the entire spectrum of coupling constant values $0<\lambda<\infty$, with specific application to the quartic AHO. Section 6 is devoted to some concluding remarks.

2. Brief remarks on summability techniques, continued fractions and hydrogenic perturbation theory

As in many situations encountered in quantum mechanics, the eigenvalue problems in Eq. (1.23) and Eq. (1.24) represent singular perturbation problems which yield Rayleigh-Schrödinger expansions with zero radius of convergence. Although divergent, RS series may be asymptotic and summable to the eigenvalues $E(\lambda)$ by techniques such as Padé approximants-continued fractions [10] or the method of Borel [11]. We outline the major ideas concerning these summability methods below.

The RS expansions studied in this paper have the generic form

$$E(\lambda)=\sum_{n=0}^{\infty} E^{(n)}\lambda^n \tag{2.1}$$

and are divergent but asymptotic to $E(\lambda)$, with the large order behavior of the $E^{(n)}$ typically given by

$$E^{(n)}=(-1)^{n+1}Ac^n\Gamma(mn+d), \qquad n\to\infty, \tag{2.2}$$

where A, c, d and m are constants, with $m=1,2,3,\dots$. For many "standard" perturbation problems, like the two classes studied here, the RS expansions in (2.1) are negative Stieltjes for $n\geq 1$ [4], i.e.

$$E^{(n)}=-(-1)^n a_n, \qquad n\geq 1, \tag{2.3}$$

where

$$a_n=\int_0^\infty x^n p(x)\,dx \tag{2.4}$$

are the positive moments of a non-negative distribution $p(x)$ on the real line, given by

$$p(x)=\frac{1}{\pi x}\,\mathrm{Im}\,E\left(-\frac{1}{x}+i0\right). \tag{2.5}$$

Motivated by a previous interest in the relationship between RSPT and continued fractions (CF), the numerical calculations in this report have concentrated on the CF summability of the renormalized series, which, as shown below, is equivalent to Padé summability. A study of other numerical methods, including Borel summability and sequence transformations is currently in progress [12]. The CF representations assume the form

$$E(\lambda)=E^{(0)}+\lambda C(\lambda), \tag{2.6a}$$

where

$$C(z)=\cfrac{c_1}{1+\cfrac{c_2 z}{1+\cdots}}. \tag{2.6b}$$

For comprehensive treatments of the theory of continued fractions, we refer the reader to [13, 14]. Further information on the relationship between CF's and RS perturbation series is to be found in Ref. [6]. For a Stieltjes series as in Eq. (2.6), the continued fraction $C(\lambda)$ in (2.6b) is an S-fraction, i.e. all coefficients c_n are positive.

In general, the CF coefficients c_n, $n=1,2,\dots,N$, may be calculated from the RS coefficients $E^{(n)}$, $n=1,\cdots,N$, by the quotient-difference (QD) algorithm [15, 13]. The terminating CF composed of the first N coefficients c_n in (1.27) is known as the Nth convergent to $C(z)$, often denoted as $w_N(z)$. It is easy to show that $w_N(z)$ is a rational function, i.e.

$$w_N(z)=\frac{A_N(z)}{B_N(z)}, \qquad N=0,1,2,\dots, \tag{2.7}$$

with $\deg(A_N(z))=[\![(N-1)/2]\!]$ and $\deg(B_N(z))=[\![N/2]\!]$, where $[\![x]\!]$ denotes "the greatest integer contained in x". When $C(z)$ represents a formal power series $P(z)$ of a function $f(z)$, then $w_{2N}(z)$ and $w_{2N+1}(z)$ are, respectively, the $[N-1, N]$ and $[N, N]$ Padé approximants [10] to the series. If the series is Stieltjes, hence $C(z)$ an S-fraction, the even and odd convergents satisfy the inequality

$$w_{2N}(z)<f(z)<w_{2N+1}(z), \qquad N=0,1,2,\dots. \tag{2.8}$$

If the series is Padé-summable, then the sequences $\{w_{2N}(z)\}$ and $\{w_{2N+1}(z)\}$ provide, respectively, lower and upper bounds to $f(z)$ which converge to it in the limit $N\to\infty$.

We now outline the Borel summability method [11], which has become quite relevant to perturbation theory since it invokes the large order behavior of the power series coefficients. Given a function $f(z)$ which is represented by the formal power series

$$a(z)=\sum_{n=0}^{\infty} a_n z^n, \tag{2.9}$$

we define its *Borel transform* as

$$B(z)=\sum_{n=0}^{\infty} \frac{a_n}{n!} z^n=\sum_{n=0}^{\infty} b_n z^n, \tag{2.10}$$

and the *inverse Borel transform* as

$$g(z)=\frac{1}{z}\int_0^{\infty} e^{-t/z} B(t)\, dt. \tag{2.11}$$

The following results constitute Watson's theorem [16, 17]. Suppose that $f(z)$ is analytic in the sectorial region $D(\lambda, R)=\{z: |z|<R,\ |\arg z|\le \pi/2+\lambda,\ 0<\lambda<\pi/2\}$ and admits the asymptotic expansion

$$f(z)\approx \sum_{n=0}^{N} a_n z^n+R_N(z), \qquad z\to 0, \tag{2.12}$$

with

$$a_n=O(n!\,\sigma^n), \tag{2.13a}$$

$$|R_N(z)|\le A\sigma^{N+1}(N+1)!\,|z|^{N+1}, \tag{2.13b}$$

uniformly for all N and z in $D(\lambda, R)$. Then

(a) $B(z)$ converges in the circle $|z|<\sigma^{-1}$ and has analytic continuation to the sector $|\arg z|<\lambda$
(b) $g(z)$ is absolutely convergent in the region $C_R=\{z: |z-R/2|<R/2\}$ and $g(z)=f(z)$ there. The asymptotic series (2.4) is said to be *Borel summable* to $f(z)$ for $z\in C_R$.

Sokal [18] has presented a variation of Watson's theorem which reduces the region necessary for analyticity of $f(z)$. If $f(z)$ is analytic in C_R and the estimates in (2.13) are satisfied uniformly in N and in $z\in C_R$ then

(a) $B(z)$ has analytic continuation from the region $|z|<\sigma^{-1}$ to the striplike region $S_\sigma=\{z: |z-w|<\sigma^{-1},\ w\in \boldsymbol{R}^+\}$;
(b) $f(z)=g(z)$ for $z\in C_R$ as before.

This result will be important in establishing the Borel summability of the renormalized series $G(\beta)$ in Eq. (1.20).

The Borel method discussed above is not directly to asymptotic series whose coefficients diverge faster than $n!$, for example $m\ge 2$ in Eq. (2.2). A generalization of this method is possible for these cases: cf. [3], p. 45.

Concerning the hydrogenic perturbation problems studied in this paper, we have employed the "so(4, 2) Lie algebra technology" [19, 20] to calculate perturbation coefficients. This method reformulates hydrogenic problems into eigenvalue problems over a discrete Sturmian basis. In this way, the problems presented by the existence of continuum states are bypassed. For problems such as (1.24), as well as Stark and Zeeman problems, each order of perturbation theory involves only a finite number of summations. Its application to the hamiltonians in (1.24) is a straightforward extension of the $p=1$ "charmonium" problem discussed in [21]. (In fact, the general case $p \geq 1$ is discussed in Sect. V of [21].)

3. Anharmonic oscillators (AHO)

Let the RS expansions for the oscillator hamiltonians in Eq. (1.23) be denoted as

$$E_K^m(\lambda) = \sum_{n=0}^{\infty} A_K^{(n),m} \lambda^n, \qquad K = 0, 1, 2, \ldots \tag{3.1}$$

where $A_K^{(n),m} = 2K+1$. Historically, a detailed analysis of the quartic AHO (QAHO), $m=2$, by Bender and Wu [22] and Simon [4] introduced the era of large order perturbation theory (LOPT). It should be mentioned that Reid [23] actually performed the first summability studies of the QAHO perturbation series several years earlier by means of continued fractions.

The large order behavior of the RS coefficients $E^{(n),m}$ was determined by Bender and Wu using WKB techniques, and can be summarized by the interesting compact formula [24]

$$A_K^{(n),m} \approx \frac{(-1)^{n+1}(m-1)2^K}{\pi^{3/2} K! 2^{2n-1}} \Gamma[(m-1)n + K + \tfrac{1}{2}] \left[\frac{\Gamma(2m/(m-1))}{\Gamma^2(m/(m-1))}\right]^{(m-1)n+1/2}. \tag{3.2}$$

(Note that this formula differs slightly from Eq. (3) in Ref. [24] since the hamiltonians in (1.23) are rescaled.) In all cases the perturbation series are divergent and asymptotic to $E_K^m(\lambda)$ in the cut plane $|\arg \lambda| < \pi$, the region of analyticity of $E_K^m(\lambda)$. The series are also negative Stieltjes for $n \geq 1$. Only for $m = 1, 2$ is the series Padé-summable in the cut plane to $E_K^m(\lambda)$. The Borel summability of the series for $m \geq 1$ has also been established [25, 26].

The infinite field expansions for these anharmonic oscillators assume the form

$$E^m(\lambda) = \lambda^{1/(m+1)} \sum_{n=0}^{\infty} F^{(n),m} \lambda^{-2n/(m+1)}, \qquad \lambda \neq 0, \tag{3.3}$$

where the $F^{(0),m}$ are the eigenvalues of the oscillators

$$\mathscr{H}^m = -\frac{d^2}{dx^2} + x^{2m}. \tag{3.4}$$

We now define the renormalized hamiltonians

$$\mathscr{H}_R^m(\beta) = -\frac{d^2}{dx^2} + x^2 + \beta(x^{2m} - x^2) = G^m(\beta) \tag{3.5}$$

and apply RSPT to produce a series expansion of $G^m(\beta)$,

$$G^m(\beta)=2K+1+\sum_{n=1}^{\infty} G^{(n),m}\beta^n. \tag{3.6}$$

Our goal is to assign a sum to (3.6) for $\beta=1$, since $G_K^m(1)=F_K^{(0),m}$. As shown below, the series is Borel summable for $\beta\in[0,1]$. There is no guarantee, however, that it is Stieltjes and Padé summable. The numerical treatments in this paper will still employ the Padé-CF methods, however, because there is good indication that the series is summable in this way.

Some caution should be exercised when employing summability techniques (especially Padé-CF) to the series in (3.6). The perturbation $\mathscr{W}=x^{2m}-x^2$ is not positive definite since it possesses negative minima at $x=\pm m^{-1/(2m-2)}$ with absolute value

$$g=m^{-1/(m-1)}-m^{-m/(m-1)}. \tag{3.7}$$

In order to ensure positive definiteness of $\mathscr{W}$ (we would like $E^{(1)}$ in Eq. (2.3) to be positive), we "shift" the perturbation upwards, rewriting Eq. (3.5) as

$$\begin{aligned}\mathscr{H}_R^m(\beta)&=-\frac{d^2}{dx^2}+x^2-\beta g+\beta(x^{2m}-x^2+g)\\&=\mathscr{H}_R^{(0),m}+\beta\mathscr{W}_R^m,\end{aligned} \tag{3.8}$$

with unperturbed eigenvalues $G_R^{(0),m}=2K+1-\beta g$. Our series expansion then assumes the form

$$G^m(\beta)=2K+1-\beta g+\sum_{n=1}^{\infty}\bar{G}^{(n),m}\beta^n \tag{3.9}$$

where $\bar{G}^{(1),m}=G^{(1)}+g$, $\bar{G}^{(n),m}=F^{(n),m}$ for $n>1$.

In order to demonstrate a relationship between the RS coefficients $A^{(n),m}$ and the renormalized coefficients $G^{(n),m}$, let us write the hamiltonian in (3.5) as

$$\mathscr{H}_R^m(\beta)=-\frac{d^2}{dx^2}+(1-\beta)x^2+\beta x^{2m}=G^m(\beta). \tag{3.10}$$

We now rescale this hamiltonian via the coordinate transformation $x\to\alpha x$, where $\alpha=(1-\beta)^{-1/4}$, to give

$$\mathscr{H}_R^m(\beta)=(1-\beta)^{1/2}\left[-\frac{d^2}{dx^2}+x^2+\frac{\beta}{(1-\beta)^{(m+1)/2}}x^{2m}\right]. \tag{3.11}$$

A comparison of (3.11) and (1.23) shows that

$$G^m(\beta)=(1-\beta)^{1/2}E^m\left(\frac{\beta}{(1-\beta)^{(m+1)/2}}\right). \tag{3.12}$$

This equation reveals the renormalization map $R:\beta\to\lambda$ which, restricted to the nonnegative real line, maps $[0,1]$ onto $[0,\infty)$.

Substituting the perturbation expansions into (3.12),

$$\sum_{n=0}^{\infty} G^{(n),m}\beta^n = \sum_{n=0}^{\infty} A^{(n),m}\beta^n(1-\beta)^{-[n(m+1)-1]/2}, \tag{3.13}$$

and using the binomial expansion formula,

$$(1-\beta)^{-\alpha} = \sum_{k=0}^{\infty} \frac{\Gamma(\alpha+k)}{\Gamma(\alpha)\Gamma(k+1)}\beta^k, \tag{3.14}$$

we equate like powers of β in (3.13) to give

$$G^{(n),m} = \sum_{k=0}^{n} \frac{\Gamma((m-1)k/2+n-1/2)}{\Gamma((m+1)k/2-1/2])\Gamma(n-k+1)} A^{(k),m}. \tag{3.15}$$

This equation defines the transformation matrix $\boldsymbol{C}$ in Eq. (1.22). We also have the result

$$G^{(n),m} = O([(m-1)n]!), \qquad n\to\infty. \tag{3.16}$$

A more precise calculation of the asymptotics for the case $m=2$ follows below.

The Borel summability of the renormalized series in (3.9) may now be established. $E^m(\lambda)$ is analytic in $|\arg\lambda|<\pi$ and the suitable branch of $\lambda=\beta(1-\beta)^{-(m+1)/2}$ is analytic in $\beta\in C_R(1)$. Hence, $G^m(\beta)$ is analytic in $C_R(1)$. An argument similar to Simon ([4], p. 128) can now be used to establish the asymptotic nature of the renormalized RS series. The asymptotics given in (3.16) then give an estimate of the error between the partial sum of the series and $G^m(\beta)$. From the conditions in Eq. (2.13), this ensures Borel summability of the series to $G^m(\beta)$ on the interval $[0,1]$.

3.1. Specific application to quartic anharmonic oscillator (m = 2)

We shall first employ Eq. (3.15) to determine the dominant large-n behavior of the renormalized series coefficients $G^{(n)}$ (we omit the $m=2$ superscript here). First, let us write the large order behavior of the $A^{(n)}$ in Eq. (3.2) in the generic form

$$A_K^{(n)} \approx (-1)^{n+1}Dc^n\Gamma(n+d), \qquad n\to\infty. \tag{3.17}$$

Now, divide both sides of (3.15) by $A^{(n)}$ and rewrite summation indices to give

$$\frac{G_K^{(n)}}{A_K^{(n)}} = \sum_{j=0}^{n} \frac{A_K^{(n-j)}}{A_K^{(n)}} \frac{\Gamma(3n/2-j/2-1/2)}{\Gamma(3n/2-3j/2-1/2)\Gamma(j+1)}. \tag{3.18}$$

In the limit $n\to\infty$, we collect the dominant contribution from each term in the summation to give

$$\frac{G_K^{(n)}}{A_K^{(n)}} = \left[\sum_{j=0}^{n}(-1)^j\left(\frac{3}{2c}\right)^j\frac{1}{j!}\right]\left(1+O\left(\frac{1}{n}\right)\right)$$
$$= e^{-3/(2c)}\left(1+O\left(\frac{1}{n}\right)\right), \qquad n\to\infty. \tag{3.19}$$

Since $c = 3/2$, we have the result

$$\frac{G_K^{(n)}}{A_K^{(n)}} = e^{-1}\left(1 + O\left(\frac{1}{n}\right)\right), \qquad n \to \infty. \tag{3.20}$$

This result has been verified numerically for several K levels. It is very similar to the relationship between RSPT and the Wick-ordered perturbation series associated with the ϕ^4 field theory, as derived by Bender and Wu (cf. Sect. VII of [7]), although not exactly the same, since the renormalizations are different.

We now present some numerical estimates of the eigenvalues $F_K^{(0)}$ of the hamiltonian $\mathscr{H}$ in Eq. (3.4), as afforded by the renormalized perturbation series. For $K = 0, 1$, the coefficients $\bar{G}_K^{(n),m}$ in Eq. (3.9) have been computed to order $n = 40$, from which the continued fraction representations

$$G_K(\beta) = 2K + 1 - \beta g + \beta C_K(\beta) \tag{3.21}$$

are then constructed. In all cases, the CF coefficients c_n are positive and the sequences $\{c_{2k}\}$ and $\{c_{2k-1}\}$ observed to increase monotonically. In Table 1 we present the values of $G_K(1)$ yielded by the convergents $w_{39}(1)$ and $w_{40}(1)$ which correspond, respectively, to [19, 19] and [19, 20] Padé approximants to the series. For comparison, the variational results of [1] are presented. The CF coefficients c_n have been calculated to order $n = 70$ and are observed to be positive. This, along with the bounding properties afforded by the convergents, as seen in Table 1, strongly suggests Stieltjes behavior and Padé-summability. This still remains to be rigorously analyzed, however.

Let us again mention that these calculations are not meant to represent definitive numerical results, but rather to demonstrate the validity of the renormalization method. Nevertheless, the results are quite accurate. The achievement of extremely accurate estimates by Padé, Borel or other summability schemes is reserved for future discussion [12]. Calculations for quartic anharmonic oscillators in higher dimensions have also been performed. The results behave in a similar fashion as above and will not be reported here.

Table 1. Estimates of eigenvalues $F_K^{(0)}$ of the one-dimensional quartic oscillator $\mathscr{H}^2$ in Eq. (3.4), as obtained from a Padé-continued fraction summation of the renormalized β-series in Eq. (3.9). The values in the final column are taken from [1]

K	[19, 19]	[19, 20]	$F_K^{(0)}$
0	1.060364	1.060359	1.060362
1	3.79965	3.79970	3.799673
2	7.4556	7.4558	7.455698
3	11.6444	11.6451	11.644745
4	16.261	16.263	16.261825
5	21.240	21.236	21.238373

4. Generalized charmonium problems

We shall denote the RS expansions for the hydrogenic hamiltonians in Eq. (1.24) as

$$E^p_{NLM}(\lambda) = -\frac{1}{2N^2} + \sum_{n=1}^{\infty} E^{(n),p}_{NLM}\lambda^n, \tag{4.1}$$

where $E^p_{NLM}(\lambda)$ represents the eigenvalue of the perturbed state $\psi_{NLM}(\lambda)$ which arises from the discrete hydrogenic eigenstate ϕ_{NLM} when the perturbation λr^p is applied. The large order behavior for the RS coefficients follows a pattern quite similar to that of the anharmonic oscillators in Eq. (3.2). The result is [21, 27]

$$E^{(n),1}_{NLM} \approx \frac{(-1)^{n+1}3^{2N}2^{2N-1}}{\pi N^3(N+L)!(N-L-1)!} \exp\left[-3N + \frac{L(L+1)}{N}\right] \times (\tfrac{3}{2}N^3)^n\Gamma(n+2N), \qquad n \to \infty, \tag{4.2a}$$

and, for $p \geq 2$,

$$E^{(n),p}_{NLM} \approx \frac{(-1)^{n+1}p2^{4N/p-2N-1}}{\pi N^3(N+L)!(N-L-1)!}\left[\frac{\Gamma(1/2+1/p)\Gamma(p+2)}{\Gamma(1/p)\Gamma(3/2)}\right]^{2N} \times c^{pn}\Gamma(pn+2N), \qquad n \to \infty, \tag{4.2b}$$

where

$$c = \frac{\Gamma(1/2+1/p)\Gamma(p+2)N^{1+2/p}}{\Gamma(1/p)\Gamma(3/2)2^{2-1/p}}.$$

In fact the oscillator problems of (1.23) and the hydrogenic problems in (1.24) are related by a nonlinear transformation of coordinates. This connection was first pointed out for the special case ($m = 2$, $p = 1$) by Johnson [28] and then derived for general radial problems by Cizek and Paldus [29]. Banerjee [30] has explicitly related the two problems (1.23) and (1.24) although the relationship between the LOPT formulas (3.2) and (4.2) is not as transparent.

The infinite field expansions for these problems are given by

$$E^p(\lambda) = \lambda^{2/(p+2)} \sum_{n=0}^{\infty} F^{(n),p}\lambda^{-n/(p+2)}, \qquad \lambda \neq 0, \tag{4.3}$$

where $F^{(0)}$ are eigenvalues of the hamiltonians

$$\mathcal{H}^p = -\tfrac{1}{2}\nabla^2 + r^p, \qquad p = 1, 2, \ldots. \tag{4.4}$$

The renormalized hamiltonians are then defined as

$$\mathcal{H}^p_R(\beta) = -\tfrac{1}{2}\nabla^2 - \frac{1}{r} + \beta\left(\frac{1}{r} + r^p\right) = G^p(\beta) \tag{4.5}$$

to which we apply RSPT, i.e.

$$G^p(\beta) = -\frac{1}{2N^2} + \sum_{n=1}^{\infty} G^{(n),p}\beta^n$$
$$= -\frac{1}{2N^2} + \Delta G(\beta). \tag{4.6}$$

Using the "so(4, 2) approach" mentioned in Sect. 2, we transform (4.5) into the perturbation equation

$$(\mathcal{T}_3 - N) + \beta(N + N^{p+2}r^{p+1}) - rN^2\Delta G(\beta) = 0. \tag{4.7}$$

The operator T_3 is defined in [21]. Note that the seemingly problematic Coulomb perturbation in (4.5) becomes a constant in (4.7), contributing only to the first-order correction.

We now proceed in a fashion similar to that in Sect. 3 in order to ascertain the relationship between the renormalized coefficients $G^{(n),p}$ and the RS coefficients $E^{(n),p}$. We may work directly on the original hamiltonian $\mathcal{H}_R^p(\beta)$ in (4.5) by first rewriting it as

$$\mathcal{H}_R^p(\beta) = -\tfrac{1}{2}\nabla^2 - \frac{(1-\beta)}{r} + \beta r^p = G^p(\beta) \tag{4.8}$$

and then scaling by $r \to \alpha r$, where $\alpha = (1-\beta)^{-1}$, to give

$$\mathcal{H}_R^p(\beta) = (1-\mu)^2\left[-\tfrac{1}{2}\nabla^2 - \frac{1}{r} + \frac{\beta}{(1-\beta)^{p+2}} r^p\right]. \tag{4.9}$$

The renormalization relation between (1.24) and (4.5) is thus given by

$$G^p(\beta) = (1-\beta)^2 E^p\left(\frac{\beta}{(1-\beta)^{p+2}}\right). \tag{4.10}$$

Analogous to Eq. (3.13) in Sect. 3, we have the equation

$$\sum_{n=0}^{\infty} G^{(n),p}\beta^n = \sum_{n=0}^{\infty} E^{(n),p}\beta^n(1-\beta)^{-[n(p+2)-2]} \tag{4.11}$$

and using the binomial expansion formula (3.14) we obtain the relationship

$$G^{(n),p} = \sum_{k=0}^{n} \frac{\Gamma((p+1)k+n-2)}{\Gamma((p+2)k-2)\Gamma(n-k+1)} E^{(k),p}. \tag{4.12}$$

This relation also implies that the renormalized coefficients $G^{(n),m}$ behave asymptotically as $O([pn]!)$. A more precise expression for the case $p = 1$ is derived below. With this results, Borel summability of the renormalized β-series follows, following our previous discussion for the case of anharmonic oscillators.

4.1. *Specific application to charmonium (p = 1)*

In the same way as for the quartic anharmonic oscillator case (cf. Eqs. (3.16–19)) we can find the large-n behavior of the renormalized series coefficients $G^{(n)}$ (omitting the superscript $p = 1$). The final result is

$$\frac{G_{NLM}^{(n)}}{E_{NLM}^{(n)}} = e^{-2/N^3}\left(1 + O\left(\frac{1}{n}\right)\right), \qquad n \to \infty. \tag{4.13}$$

Table 2. Estimates of eigenvalues $F^{(0)}_{NL0}$ of the three-dimensional "Airy hamiltonian" $\mathscr{H}^1$ in Eq. (4.4), as obtained from a Padé-continued fraction summation of the renormalized β-series in Eq. (4.6). For $L=0$, the $F^{(0)}_N$ are the negative zeros of the Airy equation, whose tabulated values are taken from [31]. For nonzero L, the values given are the numerical results of [32]

N	L	[19, 19]	[20, 20]	$F^{(0)}_{NL0}$
1	0	1.855754	1.855761	1.855757
2	0	3.24430	3.24575	3.244607
2	1	2.66781	2.66784	2.6679
3	0	4.370	4.388	4.381671
3	1	3.87673	3.87681	3.8768
3	2	3.37174	3.37182	3.3718

We now present the numerical estimates of the eigenvalues $F^{(0)}_K$ of the hamiltonian $\mathscr{H}^1$ in Eq. (4.4). (This hamiltonian defines a three-dimensional Airy eigenvalue equation.) For $N=1,2,3$, $L=0,1,\ldots,N-1$, $M=0$, the coefficients $G^{(n)}_{NLM}$ in Eq. (4.6) have been computed to order $n=40$. From these coefficients are computed the convergents $w_1,\ldots,w_{40}$ of the continued fraction representation

$$G_{NLM}(\beta)=-\frac{1}{2N^2}+\beta C(\beta) \tag{4.14}$$

evaluated at $\beta=1$. In Table 2 are given the values of $G_{NLM}(1)$ yielded by convergents w_{39} and w_{40}. For $L=0$, the eigenvalues $F^{(0)}_K$ are negative zeros of the Airy equation [9, 21] and have been tabulated [31]. Eichten et al. [32] have calculated eigenvalues for nonzero L values. As in the quartic AHO case, the CF coefficients c_n are observed to be positive, with even and odd indexed subsequences increasing monotonically. This behavior strongly suggests a Stieltjes renormalized series.

5. Calculation of perturbed eigenvalues via renormalized RSPT

The renormalized perturbation series obtained above were primarily designed to calculate the infinite field eigenvalues $F^{(0)}$. In this section we show that a "doubling rescaling" permits accurate calculation of $E(\lambda)$ for $0<\lambda<\infty$ from the original RS perturbation series. The method exploits the fact that the interval $\beta\in[0,1]$ is mapped onto the infinite interval $\lambda\in[0,\infty)$ by the renormalization relations in Eqs. (3.12) and (4.10).

We illustrate this method with a specific application to the quartic anharmonic oscillator problem, $m=2$ in Eq. (1.23). Assume we wish to calculate the eigenvalues $E(\lambda)$ of the operator

$$\mathscr{H}=-\frac{d^2}{dx^2}+x^2+\lambda x^4. \tag{5.1}$$

Applying the scaling transformation $x \to \tau^{1/2}x$, $\tau \in \boldsymbol{R}^+$ to yield the new hamiltonian

$$\mathscr{H}_\tau = -\frac{d^2}{dx^2} + \tau^2 x^2 + \lambda\tau^3 x^4 \tag{5.2}$$

with eigenvalues $\tau E(\lambda)$. Now employing the renormalized hamiltonian of Eqs. (3.8) and (3.10),

$$\mathscr{H}_R = -\frac{d^2}{dx^2} + (1-\beta)x^2 + \beta x^4, \tag{5.3}$$

with eigenvalue perturbation expansion

$$G(\beta) = 2K + 1 - \tfrac{1}{4}\beta + \sum_{n=1}^{\infty} G^{(n)}\beta_n, \tag{5.4}$$

we choose the scaling parameter τ and the renormalized coupling constant β so that the hamiltonians in (5.2) and (5.3) coincide, i.e. $\tau^2 = 1-\beta$ and $\beta = \lambda\tau^3$. This is equivalent to the condition

$$\lambda\tau^3 + \tau^2 - 1 = 0. \tag{5.5}$$

Note that for $\lambda = 0$, $\tau = 1$ and for $\lambda \to \infty$, $\tau \to 0$ as $\lambda^{-1/3}$. Moreover, for $\lambda \geq 0$ there is only one root τ of (5.5) which lies in the interval $[0, 1]$. This acceptable root ensures that $\beta \in [0, 1]$. For practical purposes, we can locate τ to prescribed accuracy using Newton's method. The eigenvalue of (5.1) is then given by

$$E(\lambda) = \tau^{-1}G(\tau^3\lambda) = \tau^{-1}G(1-\tau^2). \tag{5.6}$$

The basic procedure is then: (i) calculate the renormalized coefficients $G^{(n)}$ either from the RS coefficients $E^{(n)}$ of Eq. (5.1) or from RSPT applied to Eq. (5.3), (ii) compute τ from Eq. (5.5), (iii) "sum" the series, either by Borel or Padé and (iv) compute $E(\lambda)$ from Eq. (5.6). Here, we have constructed the continued fraction representation to the series in (5.4),

$$E(\lambda) = \tau^{-1}[2K + 1 - \tfrac{1}{4}\beta + \lambda C(\lambda)], \tag{5.7}$$

and computed its convergents $w_i(\lambda)$. Table 3 gives the estimates yielded by perturbation theory to order $n = 40$ for the levels $K = 0, 1, 2, 3$ of the quartic anharmonic oscillator. These results are compared with calculations of Biswas et al. [33] and Hioe and Montroll [34]. The maximum error in $E(\lambda)$, expected to occur in the limit $\lambda \to \infty$, will be the error in the values of the eigenvalue $F^{(0)}$ yielded, by the renormalized β-series. These errors can be determined from the results in Table 2. Also for comparison are presented the Padé–CF sums of like order to the usual RS perturbation series for $E(\lambda)$, as well as Borel–Padé summation of this series as reported in [26]. The Borel–Padé method somewhat extends the range of λ values for which eigenvalues can be extracted. Nevertheless, both low-field methods break down rapidly for even moderate values of λ.

Table 3. Estimates of ground-state eigenvalues $E_0(\lambda)$ of the one-dimensional quartic anharmonic oscillator in Eq. (5.1). $[19, 19](\tau)$ and $[19, 20](\tau)$ denote Padé approximants to the renormalized series in Eq. (5.4), with $\beta = 1 - \tau^2$, where τ is the root of Eq. (5.5). These values are compared with exact ground state energies $E_0(\lambda)$ computed in [33], except for $\lambda = 2000.0$, which is taken from [34]. The columns denoted $[i, j](\lambda)$ denote respective Padé approximants to the usual low-field RS perturbation expansion of Eq. (5.1). The final column presents the results of Borel–Padé summation of the low-field series as published in [26]

λ	$[19, 19](\tau)$	$[19, 20](\tau)$	$E_0(\lambda)$	$[19, 19](\lambda)$	$[19, 20](\lambda)$	$E_{BP}(\lambda)$
0.1	1.0625855095	1.0625855095	1.0625855095	1.0652855095	1.062855095	1.0625855095
0.5	1.2418540597	1.2418540596	1.2418540597	1.24185408	1.24185404	1.24185404 (67)
1.0	1.392351645	1.392351638	1.3923516415	1.392356	1.392348	1.392350 (6537)
2.0	1.60754135	1.60754125	1.6075413025	1.60778	1.60734	1.60750 (93)
3.0	1.7695890	1.7695886	1.7695888443	1.771	1.768	1.7694 (141)
4.0	1.9031372	1.9031367	1.9031369455	1.907	1.899	1.902 (6241)
5.0	2.0183402	2.0183411	2.0183406494	2.028	2.010	2.017 (2350)
10.0	2.4491753	2.4491728	2.4491740721	2.53	2.38	2.440 (5273)
20.0	3.009947	3.009942	3.0099448156	3.3	2.8	—
50.0	4.003998	4.003987	4.0039927683	5.5	3.2	—
100.0	4.999425	4.999409	4.9994175451	9.1	3.4	—
2000.0	13.388469	13.388413	13.3884417	—	—	—

6. Concluding remarks

We have shown that the construction of an "infinite-field" hamiltonian from a "low-field" hamiltonian is equivalent to the rescaling of spatial coordinates of the latter by a coupling constant (λ) dependent transformation. The series in the "renormalized" parameter β is related to the low-field RS expansion by an invertible linear transformation. Both series exhibit the same dominant large-order behavior. The advantage of renormalization is that the interval $\lambda \in [0, \infty)$ has been replaced by the interval $\beta \in [0, 1]$. Generally, the β series will be Borel summable in this interval. The renormalization described in this paper is similar to that obtained by a Wick-ordering in quantum field theory. This feature has also been discussed and exploited by Killingbeck [35].

It should be noted that a similar coordinate-scaling procedure was employed [36] to optimize the Löwdin method of inner projection [37] to obtain lower bounds to eigenvalues. The derivation was different, however. The scaling $x \to \tau x$ was dictated by the condition that the one-dimensional variational energy

$$\varepsilon(\tau) = \langle \phi^{(0)} | \tau^{-1} \mathscr{H}_\tau | \phi^{(0)} \rangle \tag{6.1}$$

be minimized by τ. This requirement yields the relation

$$3\lambda\tau^3 + \tau^2 - 1 = 0, \tag{6.2}$$

which is obviously different from Eq. (5.5). In fact, Eq. (6.2) represents an *optimal* renormalization by minimizing the difference between the upper estimate $\varepsilon(\tau)$ and the lower bound afforded by inner projection. Similar results have been obtained for sextic and octic [36, 38] anharmonic oscillators. A criterion similar to Eq. (6.1) has been independently employed by Cohen and Kais [39] to construct convergent series expansions of perturbed eigenvalues.

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