Journal of Mathematical Physics

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Cite as: Journal of Mathematical Physics **27**, 185 (1986); https://doi.org/10.1063/1.527360
Submitted: 30 May 1985 . Accepted: 10 July 1985 . Published Online: 04 June 1998

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Continued fractions and Rayleigh–Schrödinger perturbation theory at large order

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(Received 30 May 1985; accepted for publication 10 July 1985)

Concern with the continued fraction representations of divergent Rayleigh–Schrödinger perturbation expansions in quantum mechanics is expressed. The following relation between the large-order behavior of the continued fraction coefficients c_n and the perturbation series coefficients $E^{(n)}$ is shown to exist: If $E^{(n)} \sim (-1)^{n+1}\Gamma(pn+a)$, $p = 0,1,2,\ldots$, as $n \to \infty$, then $c_n = O(n^p)$ as $n \to \infty$. The case $p = 1$ is studied in detail here, using the problems of the quartic anharmonic oscillator and the hydrogen atom in a linear radial potential as illustrative examples. For $p = 1$ the asymptotics of the c_n are shown to be linked to the infinite field limit $E(\lambda) \sim F^{(0)}\lambda^{\alpha}$, predicting α and providing convergent estimates of $F^{(0)}$.

I. INTRODUCTION AND MOTIVATION

Perturbation methods have been an indispensible tool of applied mathematics and theoretical physics. The fundamental work of Lord Rayleigh[1] and of Schrödinger[2] provided a basis for the important quantum mechanical perturbation that bears their names. Suppose that we have a quantum mechanical system characterized by a Hamiltonian operator $\hat{H}^{(0)}$ with known energy eigenvalues $E_m^{(0)}$. Now let this system be perturbed, for example, by an external magnetic field, so that it is now represented by the Hamiltonian $\hat{H}(\lambda) = \hat{H}^{(0)} + \lambda\hat{V}$, where $\hat{V}$ represents the perturbation and λ, the coupling constant, represents its strength. The question is, "What are the eigenvalues $E_m(\lambda)$, if any, of $\hat{H}(\lambda)$?" Generally, the perturbed eigenvalue problem is not exactly solvable and approximation methods must be employed. Rayleigh–Schrödinger perturbation theory (RSPT) represents the unknown energy (and wave function) as a Taylor series in the coupling constant

$$E(\lambda) = E^{(0)} + \sum_{n=1}^{\infty} E^{(n)}\lambda^n . \tag{1.1}$$

The expansion coefficients $E^{(n)}$ are determined by well defined procedures. One of the questions of large-order perturbation theory (LOPT) is, "How do the $E^{(n)}$ behave as $n \to \infty$?"

Traditionally, physicists and chemists have been content to compute perturbation expansions to only one or two terms, for a number of reasons. In most situations, this number of terms is sufficient to remove any degeneracy of the unperturbed problem, so the physics associated with the perturbation has been revealed. Moreover, in most laboratory applications, $\lambda \ll 1$ and these terms provide good estimates of $E(\lambda)$. Another reason is that the calculation of higher-order terms, even for simple systems such as the hydrogen atom, may be very tedious. However, developments over the last twenty years have changed the status of perturbation calculations. In many physical situations, e.g., intense magnetic fields observed on the surfaces of neutron stars, the coupling constant may assume values reaching several orders of magnitude. In addition, computers have made it possible to calculate perturbation expansions for a variety of simple quantum mechanical problems to large order. Some of the oldest perturbation problems of nonrelativistic quantum mechanics, e.g., the anharmonic oscillator, the Stark and quadratic Zeeman effects in hydrogen, have been found to yield divergent perturbation series. Only relatively recently was the perturbation expansion of the classical quartic anharmonic oscillator studied in detail by Bender and Wu,[3–5] Loeffel *et al.*,[6] Simon,[7] and others. Since then, LOPT, concerned with the nature of these expansions and their summability, has evolved into an intense and ongoing area of research in mathematical, theoretical, as well as atomic and molecular physics.[8] Much of the stimulus for this research has come from quantum field theory where perturbation methods are essential. Simple perturbation problems of nonrelativistic quantum mechanics, such as those mentioned above, are similar in nature to the problems encountered in field theory. For example, the problems of the hydrogen molecule-ion and double-welled oscillators are of relevance to quantum field theories with degenerate vacuum states. Many such problems have revealed a rich mathematical structure and provide excellent testing grounds for the development of efficient and accurate summability methods.

Many of the perturbation expansions encountered in theoretical physics are divergent and their large-order behavior is given typically by

$$E^{(n)} \sim (-1)^{n+1} A\Gamma(pn+a)k^n , \quad \text{as } n \to \infty , \tag{1.2}$$

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 0022-2488/86/010185-17$02.50

where A, p, a, and k are constants. Titchmarsh[9] and Kato[10] showed many years ago that such nonconvergent expansions may still be asymptotic. In special cases the perturbation expansions may be shown to be rigorously Borel summable or, in the case of Stieltjes series, Padé summable.[11]

In this paper, we focus on continued fraction (CF) representations of the RS perturbation series in Eq. (1.1) and (1.2), having the form

$$E(\lambda)=E^{(0)}+\lambda C(\lambda)$$
$$=E^{(0)}+\cfrac{c_1\lambda}{1+\cfrac{c_2\lambda}{1+\cfrac{c_3\lambda}{1+\ddots}}} \tag{1.3}$$

The function $C(z)$ is referred to as a RITZ (rotation-inversion-translation-z) fraction.[12] More specifically, we are concerned with the large-order behavior of the c_n, which shall be abbreviated as CFLO (continued fractions at large order).

The continued fraction representations of some standard perturbation expansions whose coefficients exhibit the asymptotic behavior in (1.2) demonstrate two noteworthy features: (1) all $c_n>0$, hence $C(\lambda)$ is a Stieltjes fraction,[12] a consequence of the Stieltjes nature of the perturbation series, and (2) $c_n \sim Dn^p$, as $n\to\infty$, where D is a constant. For convenience, we refer to such continued fractions as $S_{(p)}$ fractions. The function $E(\lambda)$ is typically analytic in the cut plane $\widetilde{\mathbb{C}}=\{\lambda:|\arg\lambda|<\pi\}$, and for $p\leqslant 2$, the expression in Eq. (1.3) converges to $E(\lambda)$ uniformly on compact subsets of $\widetilde{\mathbb{C}}$. In this way, the S fraction is seen to be a much more natural representation of $E(\lambda)$ than its perturbation series counterpart.

In an earlier study,[13] this gross asymptotic connection was numerically exploited to provide very good estimates of the eigenvalue $E(\lambda)$ for rather high values of the coupling constant λ; in other words, to serve as an effective numerical summability method. Since that report, the asymptotic relation between LOPT and CFLO has been refined for a number of problems yielding $S_{(1)}$ fraction representations.[14–16] Asymptotic analysis reveals that significant information is encoded in these CF representations.

The organization of this paper is as follows: In Sec. II are presented the main features of RITZ continued fractions and their representations of formal power series, S fractions, and the Stieltjes moment problem. In Sec. III, Simon's theory of the Stieltjes nature of perturbation expansions is outlined along with a synopsis of the Bender–Wu method of determining the large-order behavior of the coefficients $E^{(n)}$. The connection between CFLO and LOPT is then discussed. In Sec. IV we look at the $S_{(1)}$ fraction representations afforded by two well-known perturbation problems: the quartic anharmonic oscillator and the hydrogen atom in a linear radial potential. The large-λ behavior for a particular class of $S_{(1)}$ fractions, including the examples cited above, is shown in Sec. V to be related to the asymptotics of the c_n. This in turn implies a relationship between CFLO and the infinite field expansion of the perturbation problem concerned. Specifically, if the infinite field expansion has the form $E(\lambda)\sim F^{(0)}\lambda^{\alpha}$, as $\lambda\to\infty$, and the c_n behave asymptotically as $c_n\sim\frac{1}{2}kn+A^{(i)}+o(1)$, as $n\to\infty$, where $i=(1,2)$, if n is (even,odd), then $\alpha=\frac{1}{2}-(A^{(1)}-A^{(2)})/k$. Moreover, asymptotic expansions of the $S_{(1)}$ fraction representations afford converging estimates of the leading coefficient $F^{(0)}$. The examples cited above will be analyzed in Sec. VI to show that a simple relationship analogous to feature (2) does not exist for subdominant terms in the CFLO and LOPT expansions. We mention that some of these results were announced in a preliminary report.[15]

II. RITZ CONTINUED FRACTION REPRESENTATIONS OF FORMAL POWER SERIES

A. RITZ fractions

In this section are outlined some important properties of the RITZ fractions defined in Eq. (1.3). Theorems are presented here without proof. Discussions and proofs can be found in the standard texts on continued fractions[17–19] and Padé approximants.[20,21] The book by Henrici[12] contains a presentation of RITZ and S fractions most relevant to this study.

The continued fraction function in Eq. (1.3), $C(z)$: $\mathbb{C}\to\mathbb{C}$, which we write in the following fashion:

$$C(z)=\frac{c_1}{1}\,\frac{}{+}\,\frac{c_2z}{1}\,\frac{}{+}\,\frac{c_3z}{1}\,\frac{}{+}\cdots, \tag{2.1}$$

and abbreviate as

$$C(z)=z^{-1}\mathop{\mathbf{K}}_{n=1}^{\infty}\frac{c_nz}{1},$$

is referred to as a RITZ (rotation-inversion-translation-z) fraction since it may be formally defined as a composition of linear fractional transformations with complex parameter z. If $C(z)$ is a *terminating fraction*, i.e., $c_k=0$ for $k>n$, then it is a rational function of z. If $C(z)$ is *nonterminating*, which is to be assumed throughout the course of this paper, it may be truncated by setting $c_k=0$, $k>n$, to produce a set of rational functions, $w_n(z)$, the nth *convergents* or *approximants* to $C(z)$,

$$w_n(z)=\frac{c_1}{1}\,\frac{}{+}\,\frac{c_2z}{1}\,\frac{}{+}\,\frac{c_3z}{1}\,\frac{}{+}\cdots\frac{}{+}\,\frac{c_nz}{1}$$
$$=\frac{A_n(z)}{B_n(z)}. \tag{2.2}$$

The polynomials $A_n(z)$ and $B_n(z)$ are the nth *numerator and denominator*, respectively, of $C(z)$. They satisfy the recurrence relations

$$A_n(z)=A_{n-1}(z)+c_nzA_{n-2}(z),$$
$$B_n(z)=B_{n-1}(z)+c_nzB_{n-2}(z),\quad n=2,3,4,..., \tag{2.3}$$

with initial values $A_0=0$, $B_0=1$, $A_1=c_1$, $B_1=1$. Moreover, it may easily be shown that $L=\deg\{A_n(z)\}=[(n-1)/2]$ and $M=\deg\{B_n(z)\}=[n/2]$, where $[x]$ denotes the greatest integer contained in x. If we let a_{nj}, $0\leqslant j\leqslant L$, and b_{nk}, $0\leqslant k\leqslant M$, represent the coefficients of x^j and x^k in the polynomials $A_n(z)$ and $B_n(z)$, respectively, then Eq. (2.3) implies the recurrence relations

$$a_{nj}=a_{n-1,j}+c_na_{n-2,j-1},\quad j=0,1,...,[(n-1)/2],$$
$$b_{nj}=b_{n-1,j}+c_nb_{n-2,j-1},\quad j=0,1,...,[n/2], \tag{2.4}$$

TABLE I. Numerator and denominator polynomial coefficients a_{nj} and b_{nj} of the RITZ fraction convergents $w_n(z)$ defined in Eq. (2.2). These coefficients are expressed in terms of the RITZ fraction coefficients c_n and obey the recursion relations in Eq. (2.4).

	$n \backslash j$	0	1	2	3
	1	c_1			
	2	c_1			
	3	c_1	c_1c_3		
a_{nj}	4	c_1	$c_1c_3 + c_1c_4$		
	5	c_1	$c_1c_3 + c_1c_4 + c_1c_5$	$c_1c_3c_5$	
	6	c_1	$c_1c_3 + c_1c_4 + c_1c_5 + c_1c_6$	$c_1c_3c_5 + c_1c_3c_6 + c_1c_4c_6$	
	7	c_1	$c_1c_3 + c_1c_4 + c_1c_5 + c_1c_6$ $+ c_1c_7$	$c_1c_3c_5 + c_1c_3c_6 + c_1c_4c_6 + c_1c_3c_7$ $+ c_1c_4c_7 + c_1c_5c_7$	$c_1c_3c_5c_7$

	$n \backslash j$	0	1	2	3
	1	1			
	2	1	c_2		
	3	1	$c_2 + c_3$		
b_{nj}	4	1	$c_2 + c_3 + c_4$	c_2c_4	
	5	1	$c_2 + c_3 + c_4 + c_5$	$c_2c_4 + c_2c_5 + c_3c_5$	
	6	1	$c_2 + c_3 + c_4 + c_5 + c_6$	$c_2c_4 + c_2c_5 + c_3c_5 + c_2c_6 + c_3c_6 + c_4c_6$	$c_2c_4c_6$
	7	1	$c_2 + c_3 + c_4 + c_5 + c_6 + c_7$	$c_2c_4 + c_2c_5 + c_3c_5 + c_2c_6 + c_3c_6 + c_4c_6$ $+ c_2c_7 + c_3c_7 + c_4c_7 + c_5c_7 + c_6c_7$	$c_2c_4c_6 + c_2c_4c_7 + c_2c_5c_7$ $+ c_3c_5c_7$

where $a_{00} = 0$, $b_{00} = 1$; $a_{0i} = b_{0i} = 0$, for $i > 0$; $a_{10} = c_1$, $b_{10} = 1$. Clearly, these polynomial coefficients are expressible solely in terms of the CF coefficients c_n. Closed-form expressions for $n \leqslant 7$ are presented in Table I.

Theorem 2.1: For each convergent $w_n(z)$ of $C(z)$, the polynomials $A_n(z)$ and $B_n(z)$ have no common zeroes.

The continued fraction $C(z)$ is said to *converge* at a point z_0 if $\lim_{n\to\infty} w_n(z_0)$ exists and is finite. Theorems which relate the regions of convergence of $C(z)$ to the behavior of the c_n are given in Refs. 17–20.

B. RITZ fractions and corresponding power series

Clearly, the approximants $w_n(z)$ in Eq. (2.2) are rational functions analytic at $z = 0$. The following theorem is important in establishing a correspondence between RITZ fractions and formal power series.

Theorem 2.2: The first n terms of the Taylor series expansions of $w_{n+k}(z)$, $k = 0,1,2,\ldots$ are identical.

The formal power series,

$$P(z) = a_0 + a_1 z + a_2 z^2 + \cdots, \tag{2.5}$$

and the continued fraction $C(z)$ are said to correspond to each other if

$$P(z) - w_n(z) = O(z^n). \tag{2.6}$$

From Eq. (2.3) this is equivalent to the condition

$$P(z) - A_n(z)/B_n(z) = O(z^{L+M+1}), \tag{2.7}$$

which is precisely the relation defining the unique $[L,M]$ Padé approximant[20,21]

$$[L,M](z) = \frac{p_0 + p_1 z + \cdots + p_L z^L}{1 + q_1 z + \cdots + q_M z^M}, \tag{2.8}$$

to the series $P(z)$. Thus $w_{2N}(z) = [N-1,N](z)$ and $w_{2N+1}(z) = [N,N](z)$ so that the sequence $\{w_n(z)\}_{n=0}^{\infty}$ generates a stepwise descent of the Padé table of $P(z)$.

Remarks: There is an immediate computational advantage afforded by RITZ representations over their Padé counterparts—a *single* sequence of RITZ coefficients c_n generates the two diagonal Padé sequences. In order to move from $w_{2N}(z)$ to $w_{2N+1}(z)$, we need only add the coefficient c_{2N+1} to the sequence $\{c_n\}_{n=1}^{2N}$. As will be shown below, this computation requires the additional series coefficient a_{2N}. This is not the situation for Padé approximants, where a new set of $L + M + 1$ coefficients need to be calculated for each $[L,M]$ Padé.

Theorem 2.3: A necessary and sufficient condition for the existence of a unique RITZ fraction representation $C(z)$ of the formal power series in Eq. (2.5) is that $P(z)$ be *normal*, i.e., that the Hankel determinants defined by $H_0^{(0)} = 1$ and

$$H_k^{(n)} = \begin{vmatrix} a_n & a_{n+1} & \cdots & a_{n+k-1} \\ a_{n+1} & a_{n+2} & \cdots & a_{n+k} \\ \vdots & \vdots & & \vdots \\ a_{n+k-1} & a_{n+k} & \cdots & a_{n+2k-2} \end{vmatrix} \tag{2.9}$$

satisfy $H_k^{(n)} \neq 0$ for $n = 0,1$ and $k = 1,2,\ldots$. The CF coefficients c_n are then given by $c_1 = a_0$ and

$$\begin{aligned} c_{2m} &= - H_m^{(1)} H_{m-1}^{(0)} / H_{m-1}^{(1)} H_m^{(0)}, \\ c_{2m+1} &= - H_{m+1}^{(0)} H_{m-1}^{(1)} / H_m^{(0)} H_m^{(1)}. \end{aligned} \tag{2.10}$$

These equations are quite unsuitable for numerical computation of the CF coefficients, however. As in the case of

Padé approximants, the evaluation of such determinants is tedious and very sensitive to the roundoff error associated with fixed point arithmetic. There exist a number of simpler, but also numerically unstable, algorithms which exploit, either directly or indirectly, the relationships between neighboring Hankel determinants to calculate the c_n. We now outline the *quotient-difference* (QD) algorithm of Rutishauser,[22] which has been employed in this study. The notation scheme employed here differs slightly from the usual one presented in books.[12,17,23]

For the power series $P(z)$ defined in Eq. (2.5), the QD algorithm defines the two-dimensional sequences e_{nm} and q_{nm} with the initial values

$$e_{n0} = 0\,, \quad n = 1,2,3,\dots\,,$$
$$q_{n1} = -a_n/a_{n-1}\,, \quad n = 1,2,\dots\,, \tag{2.11}$$

and the following recursion relations, the so-called "rhombus rules,"

$$e_{nm} = q_{n+1,m} - q_{nm} + e_{n,m-1}\,, \tag{2.12a}$$
$$q_{nm} = e_{n,m-1} q_{n,m-1}/e_{n-1,m-1}\,, \tag{2.12b}$$
$$n = 2,3,\dots\,, \quad m = 2,3,\dots,n\,.$$

These sequences are traditionally presented as a set of interwoven two-dimensional arrays known as the *QD table,* which is shown schematically in Fig. 1. Any four elements of the table which form a unit rhombus are connected by the recursion relations of (2.12).

Theorem 2.4: If the power series $P(z)$ is normal, then its RITZ fraction representation is uniquely defined by the "diagonal" elements of the QD table, i.e.,

$$C(z) = \frac{a_0}{1\,+}\;\frac{q_{11}z}{1\,+}\;\frac{e_{11}z}{1\,+}\;\frac{q_{22}z}{1\,+}\;\frac{e_{22}z}{1\,+}\;\cdots\,. \tag{2.13}$$

The QD algorithm represents a convenient method of determining the RITZ fraction representation (if it exists) of a formal power series. The first column e_{n0} is filled with zeroes, and the next column q_{n1} is filled with the negative ratios of successive power series coefficients. Equations (2.12) are then used to calculate a QD triangle outward to the diagonal as in Fig. 1. This method is known as the *forward QD algorithm*. Each additional series coefficient a_n allows the determination of an additional CF coefficient c_n. In this way a one-to-one correspondence is seen to exist between the a_n and the c_n.

The QD scheme, as other algorithms designed to calculate RITZ CF coefficients from power series coefficients, is numerically unstable by virtue of the alternating procedures of division and subtraction. Practical calculations of RITZ coefficients to large order are thus impeded by this sensitivity to roundoff error. It is found that roughly one digit of accuracy in the c_n is lost for every two orders of calculation, implying that even in IBM quadruple precision (32 significant digits), coefficients beyond about c_{60} are totally meaningless. As a result, all calculations performed in the course of this work have been accomplished with the use of a multiple-precision software routine,[24] which allows decimal numbers to be represented by arbitrarily large numbers of

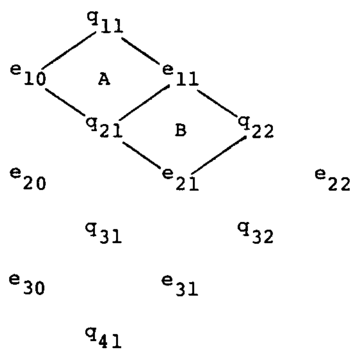

FIG. 1. The quotient-difference (QD) table, illustrating two particular unit rhombi. The elements defining rhombus A satisfy Eq. (2.12a) with $m = n = 1$. The elements of rhombus B satisfy Eq. (2.12b) with $m = n = 2$. From these equations, the rightmost elements of any rhombus may be calculated from the other three elements. The first two columns are initialized as in Eq. (2.11), permitting the calculation of the triangular lattice shown in this figure. This procedure is known as the *forward QD scheme*. The diagonal entries q_{nn} and e_{nn} define the coefficients c_n of the RITZ continued fraction representation of the formal power series concerned.

digits. In these calculations, each decimal number—including those involved in the calculation of the perturbation coefficients—was represented by, typically, 200 digits. This would ensure a 32-digit accuracy of the c_n to at least $n = 100$.

C. *S* fractions and the Stieltjes moment problem

A *Stieltjes* or *nonrational positive symmetric function* $f(z)$ may be defined by the Stieltjes integral,

$$f(z) = \int_0^\infty \frac{d\psi(t)}{1+zt}\,, \tag{2.14}$$

where $\psi(t)$ is a bounded, nondecreasing real valued function with infinitely many points of increase on $[0,\infty)$. The function $f(z)$ is said to be the Stieltjes transform of ψ, $f = \mathscr{S}\psi$, and obeys the following four basic properties: (i) $f(z)$ is analytic in the cut plane $\widetilde{\mathbb{C}} = \{z:|\arg z| < \pi\}$, (ii) $f(x) > 0$ for $x > 0$, i.e., $f(z)$ is *real positive symmetric*, (iii) if $U = \{z|\mathrm{Im}(z) > 0\}$ and $L = \{z|\mathrm{Im}(z) < 0\}$, then $f(L) \subset U$ and $f(U) \subset L$, i.e., $-f(z)$ is Herglotz,[7] and (iv) $f(z)$ admits an asymptotic expansion as $z \to 0$.

A formal expansion of the denominator of the integrand in Eq. (2.14) followed by term-by-term integration gives the series expansion

$$f(z) = \sum_{n=0}^{\infty} \mu_n z^n\,, \tag{2.15}$$

where the μ_n are real and finite moments of the measure $d\psi(t)$:

$$\mu_n = (-1)^n \int_0^\infty t^n d\psi(t)\,, \quad n = 0,1,2,\dots\,. \tag{2.16}$$

The series in Eq. (2.15), termed a *Stieltjes series*, may or may not converge for $z \neq 0$, but is asymptotic to $f(z)$ as $z \to 0$. Given a sequence of real numbers $\{\mu_n\}_{n=0}^{\infty}$, the *Stieltjes moment problem* consists of finding a real valued, bounded, and nondecreasing function $\psi(t)$ with infinitely many points of increase on $[0,\infty)$ whose moments are the μ_n.

We now define an *S* *(Stieltjes) fraction* as a nonterminating RITZ fraction of Eq. (2.1) for which $c_n > 0$, $n = 1,2,3,\ldots$.

Theorem 2.5: The RITZ fraction representation corresponding to a series of Stieltjes is an S fraction.

Theorem 2.6: The sequence of convergents $\{w_n(z)\}$ of an S fraction contains a subsequence which converges uniformly on any compact subset S of the cut plane $\tilde{\mathbb{C}}$. The limit function of this convergent subsequence will be analytic in S.

If $C(z)$ converges for $z \in S$, then $\lim_{n\to\infty} w_n(z)$ exists and all subsequences converge to the same limit function, called the *value function* (VF) of $C(z)$. If $C(z)$ does not converge for some $z \in S$, then it is possible that different subsequences of $w_n(z)$ converge to different *generalized value functions* (GVF) of $C(z)$.

Theorem 2.7: Corresponding to each GVF of an S fraction, we may construct a bounded nondecreasing function $\psi(t)$ satisfying Eq. (2.14). The function $\psi(t)$ must have an infinite number of points of increase.

Theorem 2.8: The even and odd approximants of an S fraction which corresponds to the asymptotic expansion in (2.15) obey the following bounding properties for $x > 0$:

$$w_{2N}(x) = [N-1,N](z) < f(x) < [N,N](z) = w_{2N+1}(x), \quad N = 1,2,\ldots. \tag{2.17}$$

If $C(z)$ converges, then its value function is equal to $f(z)$ for all $z \in \tilde{\mathbb{C}}$. A unique function ψ generates the moment sequence $\{\mu_n\}$ and the Stieltjes moment problem is said to be *determinate*. If $C(z)$ diverges, it will have two generalized value functions, the limits of the subsequences $w_{2n}(z)$ and $w_{2n+1}(z)$ as $n\to\infty$ and the moment problem is *indeterminate*. The convergence is uniform on every compact subset of $\tilde{\mathbb{C}}$. An infinite number of functions ψ_i yield the same moment sequence, each of which produces a Stieltjes transform, but only two of these are generalized value functions of $C(z)$. The determinacy of the moment problem is thus seen to boil down to the convergence of the S fraction $C(z)$. The following theorems are of paramount importance in the studies of LOPT and CFLO.

Theorem 2.9: An S fraction $C(z)$ whose coefficients c_n obey the relation

$$\sum_{n=1}^{\infty} c_n^{-1/2} = \infty \tag{2.18}$$

converges uniformly on all compact subsets of $\tilde{\mathbb{C}}$.

Theorem 2.10: (Carleman condition) A sufficient condition for the determinacy of the moment problem, hence the convergence of $C(z)$, is that

$$\sum_{n=1}^{\infty} |\mu_n|^{-1/2n} = \infty, \tag{2.19}$$

where the μ_n are the given moments of Eq. (2.15).

By Theorem 2.7, determinacy of the moment problem ensures Padé summability of the power series. In fact, for Stieltjes series, the Padé sequences $[N+k,N](z)$, $k = -1,0,1,\ldots$ converge in the limit as $N\to\infty$ to $f(z)$ uniformly on compact subsets of the cut plane $\tilde{\mathbb{C}}$.[20]

III. RAYLEIGH–SCHRÖDINGER PERTURBATION SERIES AND THEIR S FRACTION REPRESENTATIONS AT LARGE ORDER

We now return to the following general class of bound state eigenvalue problems: Given the unperturbed problem $\hat{H}^{(0)}\psi_m^{(0)} = E_m^{(0)}\psi_m^{(0)}$, $m = 0,1,2,\ldots$, we consider the perturbed problem

$$\begin{aligned}[\hat{H}^{(0)} + \lambda\hat{V}]\psi_m &= E_m(\lambda)\psi_m \\ &= [\hat{E}_m^{(0)} + \Delta E(\lambda)]\psi_m, \\ m &= 0,1,2,\ldots,\end{aligned} \tag{3.1}$$

where $\hat{V}$ is a positive (self-adjoint) perturbation and it is assumed that $\psi_m \to \psi_m^{(0)}$ and $\Delta E(\lambda) \to 0$ as $\lambda\to 0$. For a large number of perturbation problems, the function $\lambda^{-1}\Delta E(\lambda)$ may be shown to satisfy the four properties of a Stieltjes function given in Sec. II C. The asymptotic series to $E(\lambda)$ corresponds to the Rayleigh–Schrödinger perturbation series of Eq. (1.1). In his detailed treatment of the quartic anharmonic oscillator, Simon[7] showed that if $E(\lambda) \sim |\lambda|^q$, as $|\lambda| \to \infty$, the coefficients $E^{(n)}$ constitute a negative Stieltjes series for $n > q$. More precisely, the $E^{(n)}$ obey the dispersion relation

$$E^{(n)} = \pi^{-1}\int_{-\infty}^{0} \frac{Im(E+i0)}{\lambda^{n+1}}\,d\lambda, \quad n > q. \tag{3.2}$$

Bender–Wu theory[5] exploits Eq. (3.2) to establish the large-order behavior of the $E^{(n)}$ as $n\to\infty$. For n very large, the dominant contribution to the integral comes from the region $\lambda \sim 0$. The quantity $\mathrm{Im}(E)$ is proportional to the tunneling factor for the unstable state, whose asymptotics as $\lambda\to 0$ are determined by WKB methods. The LOPT of a number of problems has been studied in this way and it is found that typically

$$\mathrm{Im}(E+i0) \sim C(-\lambda)^b e^{B/\lambda^c}[1 + O(\lambda^d)], \quad \text{as } \lambda \to 0^-. \tag{3.3}$$

Substitution of (3.3) into (3.2) gives

$$\begin{aligned} E^{(n)} &\sim (-1)^{n+1}\frac{AB^{b/c}}{\pi c}(B^{-1/c})^n\Gamma\left(\frac{n-b}{c}\right) \\ &\quad \times [1 + O(n^{-d/c})], \\ &\quad \text{as } n\to\infty, \end{aligned} \tag{3.4}$$

which we shall write in a more general form as

$$E^{(n)} \sim (-1)^{n+1}A\Gamma(pn+a)k^n[1 + O(n^{-r})], \quad \text{as } n\to\infty, \tag{3.5}$$

where A, p, a, k, and r are constants specific to the problem studied.

From Carleman's condition in Eq. (2.19), the moment problem associated with the RS perturbation coefficients in Eq. (3.5) is guaranteed determinate for $p \leqslant 2$. Padé summability of the series is thus ensured. Borel ($p = 1$) and generalized Borel ($p > 1$) methods may also be possibly established.[11]

We now focus on the RITZ fraction representations of these generic RS perturbation series. From Eq. (3.1) and the fact that $0 < q < 1$ for many problems, we construct representations of the form

$$E_m(\lambda) = E_m^{(0)} + \lambda C^m(\lambda), \tag{3.6}$$

where

$$C^m(\lambda) = \frac{c_1^m}{1 +} \frac{c_2^m \lambda}{1 +} \frac{c_3^m \lambda}{1 +} \cdots$$

The index m represents any quantum number labeling of states and will generally be suppressed below. In these generic perturbation problems, $C(z)$ is an S fraction, i.e., $c_n > 0$ for $n = 1,2,3,\ldots$.

An interesting relationship is generally observed between the large-order behavior of the RS series coefficients $E^{(n)}$ and their S-fraction counterparts c_n. If the $E^{(n)}$ behave asymptotically as in Eq. (3.5), then

$$c_n \sim D n^p, \quad \text{as } n \to \infty, \tag{3.7}$$

where D is a constant. We shall refer to this asymptotic property as the *continued-fractions-at-large-order* (CFLO) relation. For convenience, we refer to S fractions whose coefficients behave asymptotically like (3.7) as $S_{(p)}$ fractions. The case $p = 0$ corresponds to representations of geometric power series for which the c_n approach a constant.

The behavior in Eq. (3.7) could be expected from a look at the extended QD table for the perturbation series, discussed in the Appendix. Its rows and columns grow asymptotically as $O(E^{(n+1)}/E^{(n)}) = O(n^p)$. The diagonal elements q_{nn} and e_{nn} also behave in this way as $n \to \infty$ although some work is required to obtain the coefficients of the leading term. In this paper, we restrict ourselves to an analysis of the relatively simple relation for $p = 1$, relevant to the study of $S_{(1)}$ representations presented below. The following result is proved in the Appendix.

Proposition 3.1: Given that the $E^{(n)}$ form a negative Stieltjes series for $n > 1$ and behave as in Eq. (3.5) with $p = 1$ and $r \geqslant 1$, then the coefficients of its S-fraction representation in Eq. (3.6) behave as $c_n \sim kn/2$, as $n \to \infty$.

Illustrative example—The generalized Euler series: The following modification of the classical Euler series,[12,20] $E(z) = 0! - 1!z + 2!z^2 - \cdots$, is relevant to the analysis of $S_{(1)}$ fractions presented in Sec. V:

$$F(z) = 1 + \sum_{n=1}^{\infty} (-1)^{n+1} \Gamma(n+a) k^n z^n . \tag{3.8}$$

This series has been constructed in a form which corresponds to the typical leading behavior of $n!$-type perturbation expansions [e.g., $k = 3, a = K + \frac{1}{2}$ for the QAHO series in Eq. (4.4)]. It is the asymptotic expansion of the Stieltjes transform

$$G(z) = 1 + kz \int_0^\infty \frac{e^{-t} t^a}{1 + kzt} dt \tag{3.9}$$

for $z \to 0$ in the cut plane $|\arg z| < \pi$.

The coefficients of the S-fraction representation,

$$F(z) = 1 + \frac{b_1 z}{1 +} \frac{b_2 z}{1 +} \frac{b_3 z}{1 +} \cdots, \tag{3.10}$$

are easily determined in closed form by constructing the QD table (Fig. 1) for the expansion in (3.8):

$$b_1 = k\Gamma(1+a),$$
$$b_{n,\text{even}} = \tfrac{1}{2} kn + ka, \tag{3.11}$$
$$b_{n,\text{odd}} = \tfrac{1}{2} kn - k/2 .$$

The special case $k = 1, a = 0$ corresponds to the Euler series.

The CFLO property in (3.7) provides a consistency relation between the moment conditions in Eqs. (2.8) and (2.9). In both cases, the moment problem is determinate for $p \leqslant 2$ in Eqs. (3.5) and (3.7).

From a computational viewpoint, a knowledge of $S_{(p)}$-fraction asymptotics for $p = 1,2$ has proven useful[13] in the estimation of energy eigenvalues $E(\lambda)$ for rather larger values of the coupling constant λ. For $S_{(1)}$ fractions, an extrapolation of a small number of accurately known c_n, produces an approximate "tail" of $C(\lambda)$. The approximants $w_n(\lambda)$ associated with this CF are then evaluated to sufficiently high order to ensure convergence of the fraction, i.e., $|w_{n+1}(\lambda) - w_n(\lambda)| < \epsilon$ for a given $\epsilon > 0$. Excellent estimates of $E(\lambda)$ for large λ are obtained. In the case of $S_{(2)}$ fractions, a similar extrapolation of the c_n is performed. The convergence of the $w_n(\lambda)$ is extremely slow. A suitably constructed extrapolation of even (lower bound) and odd (upper bound) approximants yields a common limit which again approximates $E(\lambda)$ very well for even large λ. Some numerical results are presented in Ref. 13.

We mention that the importance of CFLO has already been realized for the case of $S_{(0)}$ fractions, i.e., $c_n \to a$, as $n \to \infty$, where a is a constant. These types of fractions have been encountered in solid state physics[25,26] in the approximation of densities of states of periodic and aperiodic systems as well as in atomic and molecular physics[27,28] for the determination of optical dispersion profiles. In both cases, one is interested in the location of a branch cut of singularities in the complex energy plane as well as the discontinuity across the cut. The asymptotic value a is important in light of an extension of a theorem due to Van Vleck.[18]

Theorem 3.1: Let $C(z)$ be an S fraction such that $\lim_{n\to\infty} c_n = a \neq 0$, where a is a complex constant and let $\mathbb{C}_a = \{z : |\arg(az + \frac{1}{4})| < \pi\}$. The continued fraction $C(z)$ converges to a function $f(z)$, which is either meromorphic in $\mathbb{C}_a$ or identically infinity.

The region $\mathbb{C}_a$ represents the complex plane $\mathbb{C}$ cut along the line which passes through the point $z_c = -(4a)^{-1}$ and the origin. The cut begins at the point z_c and extends outward to infinity. In the context of photoabsorption studies,[28] the continued fraction corresponding to the Stieltjes series for complex polarizability $\alpha(z)$ (having nonzero radius of convergence) is constructed and the (real) asymptotic value a is estimated. The distance from the origin to the cut, $|z_c|$, corresponds to the *photoionization threshold frequency* for the atomic or molecular system concerned.

The subject of $S_{(0)}$ representations of perturbation series, including the well-known problem of a rigid dipole rotor in an electric field, will be discussed in a future report.

TABLE II. The first 105 coefficients c_n of the S-fraction representation, Eq. (4.4), of the ground-state Rayleigh–Schrödinger perturbation series for the energy $E(\lambda)$ of the quartic anharmonic oscillator in Eq. (4.1).

n	c_n	n	c_n
1	0.750 000 000 000 000 000 000 000 000 000 D + 00	54	0.406 586 405 522 041 706 283 769 067 693 D + 02
2	0.175 000 000 000 000 000 000 000 000 000 D + 01	55	0.411 421 268 655 535 125 766 943 934 596 D + 02
3	0.221 428 571 428 571 428 571 428 571 421 D + 01	56	0.421 580 132 542 199 212 702 235 748 957 D + 02
4	0.328 067 396 313 364 055 299 539 170 507 D + 01	57	0.426 418 233 947 834 481 230 612 157 025 D + 02
5	0.368 842 779 459 679 897 367 783 849 295 D + 01	58	0.436 574 196 271 822 690 130 688 022 839 D + 02
6	0.473 804 188 521 881 063 707 142 639 340 D + 01	59	0.441 415 356 393 589 419 024 936 020 957 D + 02
7	0.517 612 209 347 468 499 579 930 828 597 D + 01	60	0.451 568 567 683 689 989 026 434 041 269 D + 02
8	0.622 046 670 654 721 646 752 711 278 894 D + 01	61	0.456 412 622 835 465 321 760 882 311 956 D + 02
9	0.666 893 242 501 742 590 748 909 803 938 D + 01	62	0.466 563 221 133 621 513 614 705 133 795 D + 02
10	0.770 863 415 363 561 254 700 818 557 412 D + 01	63	0.471 410 021 611 420 740 202 843 289 912 D + 02
11	0.816 435 361 582 525 381 761 294 381 692 D + 01	64	0.481 558 133 870 169 732 229 550 002 981 D + 02
12	0.920 033 250 189 205 270 860 568 794 018 D + 01	65	0.486 407 542 342 811 785 880 668 124 362 D + 02
13	0.966 091 975 248 318 987 231 089 675 743 D + 01	66	0.496 553 285 628 456 366 775 785 329 355 D + 02
14	0.106 941 039 059 420 442 884 222 717 620 D + 02	67	0.501 405 175 758 083 127 125 447 075 667 D + 02
15	0.111 582 703 907 225 187 463 106 182 106 D + 02	68	0.511 548 658 291 584 962 866 225 233 352 D + 02
16	0.121 891 786 716 627 292 093 981 465 150 D + 02	69	0.516 402 913 545 210 988 616 740 602 626 D + 02
17	0.126 561 481 600 439 307 617 042 237 015 D + 02	70	0.526 544 235 606 717 905 492 047 637 396 D + 02
18	0.136 851 666 800 951 687 340 583 597 644 D + 02	71	0.531 400 748 227 523 481 657 986 922 305 D + 02
19	0.141 543 905 856 510 535 100 790 729 557 D + 02	72	0.541 540 002 945 683 876 082 634 129 675 D + 02
20	0.151 818 201 881 278 086 509 898 007 004 D + 02	73	0.546 398 673 058 640 534 948 768 719 363 D + 02
21	0.156 529 036 609 641 454 734 415 308 722 D + 02	74	0.556 535 947 102 096 253 126 954 317 229 D + 02
22	0.166 789 725 929 183 986 105 190 000 238 D + 02	75	0.561 396 681 933 142 450 130 413 395 460 D + 02
23	0.171 516 250 463 633 149 014 914 506 289 D + 02	76	0.571 532 056 118 585 474 617 123 149 510 D + 02
24	0.181 765 110 007 862 677 187 948 391 759 D + 02	77	0.576 394 769 310 252 475 830 880 035 511 D + 02
25	0.186 505 099 422 477 445 005 670 089 919 D + 02	78	0.586 528 319 139 005 802 204 136 059 178 D + 02
26	0.196 743 558 645 901 433 503 889 886 225 D + 02	79	0.591 392 930 148 347 636 208 678 651 578 D + 02
27	0.201 495 258 388 647 959 134 768 165 616 D + 02	80	0.601 524 726 281 461 064 295 401 471 352 D + 02
28	0.211 724 487 343 025 978 350 805 140 175 D + 02	81	0.606 391 159 848 526 671 653 170 951 027 D + 02
29	0.216 486 487 913 904 719 665 323 624 721 D + 02	82	0.616 521 268 528 770 627 915 137 953 121 D + 02
30	0.226 707 455 165 976 782 269 398 642 140 D + 02	83	0.621 389 454 205 790 738 151 998 196 930 D + 02
31	0.231 478 606 456 887 946 340 101 511 963 D + 02	84	0.631 517 937 633 613 814 640 723 299 693 D + 02
32	0.241 692 123 421 839 163 178 236 803 349 D + 02	85	0.636 387 809 366 651 971 458 620 241 430 D + 02
33	0.246 471 472 775 375 599 234 607 439 973 D + 02	86	0.646 514 726 036 083 720 705 508 426 670 D + 02
34	0.256 678 227 429 547 402 476 297 926 381 D + 02	87	0.651 386 221 792 192 662 882 270 236 493 D + 02
35	0.261 464 975 059 643 661 428 067 741 878 D + 02	88	0.661 511 626 791 776 902 003 228 269 454 D + 02
36	0.271 665 556 836 904 330 890 567 928 711 D + 02	89	0.666 384 688 225 765 166 563 320 358 766 D + 02
37	0.276 459 023 629 938 404 499 119 327 073 D + 02	90	0.676 508 633 508 864 441 634 996 399 357 D + 02
38	0.286 653 941 970 252 042 903 449 281 275 D + 02	91	0.681 383 205 664 658 379 358 696 010 237 D + 02
39	0.291 453 545 655 385 564 489 559 777 508 D + 02	92	0.691 505 740 292 848 656 085 278 687 390 D + 02
40	0.301 643 244 245 166 299 113 381 212 607 D + 02	93	0.696 381 771 335 167 227 892 366 108 653 D + 02
41	0.306 448 481 268 505 030 447 360 406 552 D + 02	94	0.706 502 941 697 920 626 433 180 581 495 D + 02
42	0.316 633 349 237 015 931 994 160 481 653 D + 02	95	0.711 380 382 670 592 101 404 492 697 713 D + 02
43	0.321 443 780 714 774 978 038 609 561 019 D + 02	96	0.721 500 232 684 006 573 528 150 279 693 D + 02
44	0.331 624 161 540 972 554 682 971 634 140 D + 02	97	0.726 379 037 291 769 538 599 407 518 198 D + 02
45	0.336 439 402 247 503 199 580 128 679 770 D + 02	98	0.736 497 608 578 733 388 621 936 009 027 D + 02
46	0.346 615 600 894 529 650 256 854 210 487 D + 02	99	0.741 377 732 989 796 844 663 583 318 223 D + 02
47	0.351 435 310 544 054 420 561 746 757 623 D + 02	100	0.751 495 065 043 661 298 463 454 064 922 D + 02
48	0.361 607 599 219 648 367 281 669 394 216 D + 02	101	0.756 376 467 710 664 171 010 360 108 025 D + 02
49	0.366 431 475 489 866 424 186 492 282 574 D + 02	102	0.766 492 598 044 229 348 950 781 251 158 D + 02
50	0.376 600 098 342 814 395 223 790 757 194 D + 02	103	0.771 375 239 541 549 915 310 285 838 617 D + 02
51	0.381 427 871 230 572 481 752 179 401 097 D + 02	104	0.781 490 203 822 940 836 992 120 212 793 D + 02
52	0.391 593 048 217 481 625 609 338 844 893 D + 02	105	0.786 374 046 698 570 669 023 801 627 046 D + 02
53	0.396 424 475 425 589 626 214 906 981 943 D + 02		

IV. $S_{(1)}$-FRACTION REPRESENTATIONS OF THE QUARTIC ANHARMONIC OSCILLATOR AND CHARMONIUM PERTURBATION SERIES

In this section we focus on two perturbation problems whose Rayleigh–Schrödinger expansions yield $S_{(1)}$-fraction representations: (1) the quartic anharmonic oscillator (QAHO) and (2) the hydrogen atom in a linear radial potential or the charmonium model. The LOPT of these expansions is known. In both cases, the S-fraction coefficients for the first few bound state levels have been computed accurately to high order, typically $n = 100$, to facilitate numerical analysis of their asymptotic behavior. Details of numerical aspects are presented in Refs. 13, 15, and 16.

A. The quartic anharmonic oscillator

The quartic anharmonic oscillator, whose perturbation expansions were first studied in detail by Bender and Wu[3–5] (with a different normalization), Loeffel *et al.*,[6] and Simon,[7] is given by the eigenvalue problem

$$\left[-\frac{d^2}{dx^2}+x^2+\beta x^4-E(\beta)\right]\psi(x)=0\,, \tag{4.1}$$

with boundary conditions $\psi(x)\to 0$, $|x|\to\infty$, $x\in\mathbf{R}$. The unperturbed eigenvalues are given by $E_K^{(0)}=2K+1$, $K=0,1,2,\ldots$. The perturbation expansion for the Kth level of Eq. (4.1) will be denoted by

$$E_K(\beta)=2K+1+\sum_{n=1}^{\infty}E_K^{(n)}\beta^n\,. \tag{4.2}$$

The large-order behavior of the RS coefficients is given by[4]

$$E_K^{(n)}\sim(-1)^{n+1}\frac{12^K}{K!}\left(\frac{6}{\pi^3}\right)^{1/2}\Gamma(n+K+\tfrac{1}{2})\,(\tfrac{3}{2})^n \times\left[1-\frac{1}{n}\left(\frac{95}{72}+\frac{29}{12}K+\frac{17}{12}K^2\right)+O\left(\frac{1}{n^2}\right)\right]. \tag{4.3}$$

The perturbation series is negative Stieltjes[7] for $n>1$. This guarantees its Padé, hence S fraction, summability to $E_K(\beta)$ in the cut plane $|\arg\beta|<\pi$.

We now consider S-fraction representations of the QAHO perturbation series having the form

$$E_K(\beta)=E_K^{(0)}+\beta C^K(\beta)\,, \tag{4.4}$$

where

$$C^K(\beta)=\frac{c_1^K}{1}\,\frac{}{+}\,\frac{c_2^K\beta}{1}\,\frac{}{+}\,\frac{c_3^K\beta}{1}\,\frac{}{+}\,\cdots\,. \tag{4.5}$$

The coefficients c_n^K have been calculated from the RS coefficients $E_K^{(n)}$ to $n=100$ for the levels $K=1$, 2, and 3. The first 100 coefficients for the ground state, $K=0$, are presented in Table II, accurate to all digits shown.

From Eq. (3.7) it is expected that $c_n^K\sim\frac{3}{4}n$, as $n\to\infty$, which is observed numerically. On the basis of more detailed numerical analysis,[14,15] the asymptotic behavior of the c_n^K is conjectured to be

$$c_n^K\sim\tfrac{3}{4}(n+K)\pm\tfrac{1}{8}+R_n^{(i)},\quad i=\begin{cases}1, & n\text{ even},\\ 2, & n\text{ odd},\end{cases} \tag{4.6}$$

where $R_n^{(i)}\to 0$, as $n\to\infty$, and it is conjectured that $R_n^{(i)}=O(n^{-1/2})$. The constant terms in Eq. (4.6) are not *a priori* correction terms—in fact, no general asymptotic expansion beyond the leading term is guaranteed. Nevertheless, numerical analysis strongly suggests these terms. Moreover, the analysis in Sec. V attests to their validity.

Before concluding this discussion, we mention that Reid[29] performed the first calculation of continued fraction representations of QAHO perturbation series. His calculations appeared well before Refs. 3–7, the latter two of which established the Stieltjes nature and Padé summability of the series. Reid did, however, realize the power of continued fraction summability of divergent Stieltjes series, using the classical Euler series as an example. His representations involved *J fractions*,[17,18] having the form

$$E_K(\beta)=E_K^{(0)}+J^k(\beta) =E_K^{(0)}+\frac{a_1\beta}{1+b_1\beta-}\,\frac{a_2\beta^2}{1+b_2\beta-}\,\frac{a_3\beta^2}{1+b_3\beta\cdots}\,. \tag{4.7}$$

The coefficients a_i, b_i, $i=1,2,\ldots,10$, were calculated for a number of levels in multiple precision and, for all cases, were found to be positive.

The J fraction in Eq. (4.7) is actually the *even part* of the S fraction in Eq. (4.5).[12] Its sequence of approximants coincides with the approximants of even order, $w_{2n}(\beta)$, of the S fraction. This fact is revealed in Reid's calculations of the first ten approximants of the J fraction for various values of β. All sequences of approximants approach the exact values $E(\beta)$ monotonically from below. The coefficients a_k and b_k are related to the c_n as follows:

$$a_1=c_1\,,\quad b_1=c_2\,,$$
$$a_i=c_ic_{i+1}\,,\quad b_i=c_{i+1}+c_{i+2}\,,\quad i=2,3,4,\ldots\,. \tag{4.8}$$

The calculation of a_i and b_i to $i=10$ is thus seen to be equivalent to determining the c_n to c_{20}. A look at the tables of J-fraction coefficients presented by Reid reveals that the a_i grow quadratically and that the b_i grow linearly, in accordance with Eqs. (4.6) and (4.8).

B. Charmonium—The hydrogen atom in a linear radial potential

The problem of a hydrogenic atom in a linear radial potential, one of many nonrelativistic quark-confinement models,[30–32] is given by the Hamiltonian (in atomic units)

$$\hat{H}(\lambda)=-\tfrac{1}{2}\nabla^2-Z/r+\lambda r\,. \tag{4.9}$$

With no loss of generality, we consider the problem for $Z=1$. The RS perturbation expansion for the energy of a given level will be denoted by

$$E_{NLM}(\lambda)=-\frac{1}{2N^2}+\sum_{n=1}^{\infty}E_{NLM}^{(0)}\lambda^n\,. \tag{4.10}$$

The indices N, L, and M denote, respectively, the principal, orbital-angular momentum, and magnetic quantum numbers of the unperturbed hydrogenic state giving rise to the level.

The large-order behavior of the RS coefficients is given by[16]

$$E_{NLM}^{(n)}\sim\frac{(-1)^{n+1}3^{2N}2^{2N-1}\exp[-3N+L(L+1)/N]}{\pi N^3(N+L)!(N-L-1)!} \times(\tfrac{3}{2}N^3)^n\Gamma(n+2N)[1+A/n+O(n^{-2})] \tag{4.11}$$

The coefficient A has been computed for a number of states but no general formula has been conjectured. The numerical evidence strongly indicates that for the S-wave states, i.e., $L=M=0$,

$$A=-\tfrac{1}{6}(21N^2+18N+10)\,. \tag{4.12}$$

The coefficients form a negative Stieltjes series[16] for $n>1$.

We now consider S-fraction representations to the charmonium series having the same form as Eq. (4.5), and let c_n^{NLM} denote the CF coefficients. These coefficients have been calculated to at least 32 digit precision to order $n = 100$ for the hydrogenic states $N \leqslant 3$, $0 \leqslant L \leqslant N-1$, $M = 0$. From Eq. (4.11) and Proposition 3.1, it is expected that $c_n \sim \frac{3}{4} N_n^3$, as $n \to \infty$, which is observed numerically. A more detailed numerical analysis[16] leads to the following conjectured behavior for the S-fraction coefficients:

$$c_n^{NLM} \sim \tfrac{3}{4} N^3(n+2N) - \tfrac{1}{2} N^3 + R_n^{(1),NLM}, \quad n \text{ even}, \tag{4.13}$$

$$c_n^{NLM} \sim \tfrac{3}{4} N^3(n+2N) - \tfrac{1}{4} N^3 + R_n^{(2),NLM}, \quad n \text{ odd},$$

where $R_n^{(i)} \to 0$, as $n \to \infty$. As in the case of the QAHO, numerical extrapolation techniques strongly suggest that the $R_n^{(i)} = O(n^{-1/2})$.

V. ASYMPTOTICS OF $S_{(1)}$ FRACTIONS AND THE INFINITE FIELD LIMIT

A. General formulation

The infinite field expansion for many standard perturbation problems assumes the form

$$E(\lambda) \sim \lambda^{\alpha} \sum_{n=0} F^{(0)} \lambda^{-n\gamma}, \quad \text{as } |\lambda| \to \infty, \tag{5.1}$$

and may often be obtained by real-valued dilation transformations, usually referred to as Symanzik transformations.[7] For example, in the case of generalized anharmonic oscillators, where $\hat{H}_m = \hat{p}^2 + x^2 + \lambda x^{2m}$, $m = 2,3,4,\ldots$, the scaling transformation $x = rx$, r real, yields $\alpha = 1/(m+1)$, $\gamma = 2/(m+1)$. The leading term coefficients $F_K^{(0)}$ represent the K th eigenvalues of the oscillator with Hamiltonian $\hat{H} = \hat{p}^2 + x^{2m}$.

The infinite field limit is reflected in the large-order behavior of certain $S_{(1)}$-fraction representations. In the examples below, for which

$$c_n \sim \tfrac{1}{2} kn + A^{(i)} + o(1), \quad i = \begin{cases} 1, & n \text{ even}, \\ 2, & n \text{ odd}, \end{cases} \tag{5.2}$$

where the $A^{(i)}$ are constants, it will be shown that the exponent α in Eq. (5.1) is given by

$$\alpha = \tfrac{1}{2} - \Delta A / k, \tag{5.3}$$

where

$$\Delta A = A^{(1)} - A^{(2)}. \tag{5.4}$$

First, consider the continued fraction

$$\widetilde{w}_{N-1}(z) = \frac{c_1}{1} + \frac{c_2 z}{1} + \cdots + \frac{c_{N-1} z g_N(z)}{1}, \tag{5.5}$$

where

$$g_N(z) = \frac{1}{1} + \frac{\tilde{c}_N z}{1} + \frac{\tilde{c}_{N+1} z}{1} + \cdots, \tag{5.6}$$

and

$$\tilde{c}_n = \tfrac{1}{2} kn + A^{(i)}, \quad n \geqslant N. \tag{5.7}$$

In other words, $\widetilde{w}(z)$ is constructed by replacing the infinite tail of $C(z)$ with one whose coefficients $\tilde{c}_n$ ignore the terms of $R_n^{(i)}$ in Eq. (5.2). For N even, we produce the *odd convergent approximation* $\widetilde{w}_{N-1}(z)$ to $C(z)$; for N odd we produce the *even convergent approximation*.

The function $g_N(z)$ in Eq. (5.6) is an $S_{(1)}$ fraction formally representing a Stieltjes transform and converging uniformly to it over compact subsets of the cut plane $\widetilde{\mathbb{C}}$. We first determine the asymptotics of $g_N(z)$ as $|z| \to \infty$, $z \in \widetilde{\mathbb{C}}$, by means of the following classical relation[17,21] between contiguous Gauss hypergeometric functions:

$$\frac{{}_2F_0(a,b+1,-z)}{{}_2F_0(a,b,-z)} = \frac{1}{1} + \frac{az}{1} + \frac{(b+1)z}{1} + \frac{(a+1)z}{1} + \cdots, \tag{5.8}$$

where $a \notin [0,1,2,\ldots]$ and $b \notin [-1,-2,\ldots]$. The ratio of the two series on the left-hand side of Eq. (5.8) formally represents the function

$$G(z) = \frac{\int_0^\infty (e^{-t} t^{a-1}/(1+zt)^{b+1})\, dt}{\int_0^\infty (e^{-t} t^{a-1}/(1+zt)^{b})}, \tag{5.9}$$

which is analytic for $z \in \widetilde{\mathbb{C}}$, provided that $\mathrm{Re}(a) > 0$. By Theorem 2.8 the S fraction in Eq. (5.8) converges uniformly to $G(z)$ on $\widetilde{\mathbb{C}}$. We now analyze the odd and even truncations individually.

Odd convergent truncation, $N=2n$: From Eqs. (5.6) and (5.7), it follows that

$$g_{2n}(z) = \frac{{}_2F_0(n + A^{(1)}/k, n + \frac{1}{2} + A^{(2)}/k; -kz)}{{}_2F_0(n + A^{(1)}/k, n - \frac{1}{2} + A^{(2)}/k; -kz)} \tag{5.10}$$

$$= \frac{U(n + A^{(1)}/k, \frac{1}{2} + \Delta A/k; (kz)^{-1})}{U(n + A^{(1)}/k, \frac{3}{2} + \Delta A/k; (kz)^{-1})}, \tag{5.11}$$

where $U(a,b;z)$ is a solution of Kummer's confluent hypergeometric equation,[33,34]

$$z \frac{d^2 w}{dz^2} + (b - z) \frac{dw}{dz} - aw = 0. \tag{5.12}$$

We now employ the relation[34]

$$U(a,b;x) = \frac{\Gamma(1-b)}{\Gamma(1+a-b)} \, {}_1F_1(a;b;x) + \frac{\Gamma(b-1)}{\Gamma(a)} x^{1-b} \, {}_1F_1(1+a-b; 2-b; x), \quad x \in \widetilde{\mathbb{C}}, \tag{5.13}$$

to expand the Kummer functions in Eq. (5.11) for $x = (kz)^{-1} \to 0^+$. The leading asymptotic behavior of the $U(a,b;x)$, in terms of the arguments a and b, is tabulated in Refs. 33 and 34. However, Eq. (5.13) is useful for the calculation of more terms in the asymptotic expansion. One special case requires care: For $b = 1$,

$$U(a,b;x) \sim -[1/\Gamma(a)][\ln(z) + \psi(a)] + O(|z \ln(z)|), \tag{5.14}$$

where $\psi(x)$ denotes the psi (digamma) function.[35] Temporarily ignoring this case, we rewrite Eq. (5.11) as

$$g_{2n}(z) = \frac{\Sigma_{i=1} p_i z^{-a(i)}}{\Sigma_{i=1} q_i z^{-b(i)}}, \tag{5.15}$$

where $0 < a(1) < a(2) < \cdots$, and $0 < b(1) < b(2) \cdots$. Clearly, these exponents are sensitive to the values of a and b in Eq. (5.13), which are, in turn, defined by the asymptotic coefficients in Eqs. (5.2) and (5.4).

Formal division in Eq. (5.15) yields the relation

$$g_{2n}(z) = D_1^{(2n)} z^{r(1)} + D_2^{(2n)} z^{r(2)}, \quad |z| \to \infty, \quad z \in \widetilde{\mathbb{C}}, \qquad (5.16)$$

where $r(1) = b(1) - a(1) > r(2) > r(3) \cdots$. Only two terms of the expansion in (5.15) are used since two terms in the expansion of the c_n, cf. (5.7), are employed.

The function $\widetilde{w}_{N-1}(z)$ in Eq. (5.5) may be interpreted as a terminating fraction—the generalized odd approximant $\widetilde{w}_{2n-1}(z)$ which may be written as

$$\widetilde{w}_{2n-1}(z) = \frac{A_{2n-2}(z) + c_{2n-1} z g_{2n}(z) A_{2n-3}(z)}{B_{2n-2}(z) + c_{2n-1} z g_{2n}(z) B_{2n-3}(z)}. \qquad (5.17)$$

The $A_k(z)$ and $B_k(z)$, $k < 2n-2$ are, respectively, the lower-order partial numerators and denominators of $C(z)$. We now expand these polynomials in terms of the coefficients in (2.4) and substitute Eq. (5.16) into Eq. (5.17). Formal multiplication of powers in z, rearrangement of terms, and subsequent division yields an expansion of the form

$$\widetilde{w}_{2n-1}(z) = W_1^{(2n-1)} z^{u(1)} + W_2^{(2n-1)} z^{u(2)} + \cdots, \quad \text{as } |z| \to \infty, \qquad (5.18)$$

where $u(1) > u(2) > \cdots$. Substitution of Eq. (5.18) into Eq. (5.5) produces the approximation

$$\widetilde{E}_{2n-1}(z) = E^{(0)} + W_1^{(2n-1)} z^{u(1)+1} + W_2^{(2n-1)} z^{u(2)+1} + \cdots, \quad \text{as } |z| \to \infty, \qquad (5.19)$$

for $z \in \widetilde{\mathbb{C}}$.

Even convergent truncation, $N = 2n+1$: In this case it follows from Eqs. (5.6) and (5.7) that

$$g_{2n+1}(z) = \frac{{}_2F_0(n+\frac{1}{2}+A^{(2)}/k, n+1+A^{(1)}/k; -kz)}{{}_2F_0(n+\frac{1}{2}+A^{(2)}/k, n+A^{(1)}/k; -kz)} \qquad (5.20)$$

$$= \frac{U(n+\frac{1}{2}+A^{(2)}/k, \frac{1}{2}-\Delta A/k; (kz)^{-1})}{U(n+\frac{1}{2}+A^{(2)}/k, \frac{3}{2}-\Delta A/k; (kz)^{-1})} \qquad (5.21)$$

Proceeding in the same manner as above, we expand the Kummer functions in Eq. (5.21) to ultimately obtain an asymptotic series for $g_{2n+1}(z)$ analogous to Eq. (5.16),

$$g_{2n+1}(z) = D_1^{(2n+1)} z^{s(1)} + D_2^{(2n+1)} z^{s(2)} + \cdots, \quad \text{as } |z| \to \infty, \quad z \in \widetilde{\mathbb{C}}, \qquad (5.22)$$

where $s(1) > s(2) > \cdots$. The function $\widetilde{w}_{N-1}(z)$ in Eq. (5.5) is now written as a generalized even approximant $\widetilde{w}_{2n}(z)$ [replace $2n-1$ by $2n$, etc., in Eq. (5.17)]. This ratio of two series again yields an expansion analogous to Eq. (5.18),

$$\widetilde{w}_{2n}(z) = W_1^{(2n)} z^{v(1)} + W_2^{(2n)} z^{v(2)} + \cdots, \quad \text{as } |z| \to \infty, \qquad (5.23)$$

where $v(1) > v(2) \cdots$. When substituted into Eq. (5.5), Eq. (5.23) yields the approximation

$$\widetilde{E}_{2n}(z) = E^{(0)} + W_1^{(2n)} z^{v(1)+1} + W_2^{(2n)} z^{v(2)+1} + \cdots, \quad \text{as } |z| \to \infty, \qquad (5.24)$$

where $z \in \widetilde{\mathbb{C}}$.

Several remarks concerning the above truncations are now to be made. First, the expansion for $g_{2n+1}(z)$ in (4.22) could also have been derived from that of $g_{2n}(z)$ in (4.16) (or *vice versa*) by using the defining property

$$g_{2n}(z) = [1 + \tilde{c}_{2n} z g_{2n+1}(z)]^{-1}$$
$$= [1 + (kn + A^{(1)}) z g_{2n+1}(z)]^{-1}. \qquad (5.25)$$

Both leading exponents in (5.16) and (5.22) satisfy the inequality $-1 < x < 0$. Furthermore, from (5.25), the exponents in these two expansions obey the relations $r(1) = -1 - s(1)$, $r(2) = -1 - 2s(1) - s(2)$. Additional manipulation reveals that expansions (5.19) and (5.24) possess the same power-law behavior, i.e.,

$$u(1) = v(1), \quad u(2) = v(2). \qquad (5.26)$$

We now consider the approximate convergents of Eqs. (5.19) and (5.24), written in the more general form

$$\widetilde{E}_N(z) = E^{(0)} + z \widetilde{w}_N(z). \qquad (5.27)$$

Their asymptotic expansions will be denoted by

$$\widetilde{E}_N(z) \sim E^{(0)} + W_1^{(N)} z^{\mu(1)} + W_2^{(N)} z^{\mu(2)} + \cdots, \quad \text{as } |z| \to \infty, \qquad (5.28)$$

where $\mu(1) = u(1) + 1$ and $\mu(2) = u(2) + 1$. As N increases, i.e., as the infinite tail of the true $S_{(1)}$ fraction is replaced farther down, better estimates of $E(z)$ are obtained. This is expressed more precisely in the following theorem.

Theorem 5.1: The approximate convergents $\widetilde{E}_N(z)$ in (5.28) converge uniformly to $E(z)$ over compact subsets of the cut plane $\widetilde{\mathbb{C}}$.

Proof: Consider the $S_{(1)}$-fraction representations of the RS perturbation series having the form $E(z) = E^{(0)} + zC(z)$. The approximants $w_n(z)$ of $C(z)$ converge uniformly to an analytic function $f(z)$ on compact subsets of $\widetilde{\mathbb{C}}$. Moreover, the bounding properties in Eq. (2.17) hold on the positive real axis. The $\widetilde{w}_N(z)$ defined in Eq. (5.5) are $S_{(1)}$ fractions analytic in the cut plane $\widetilde{\mathbb{C}}$. The functions $g_N(z)$ in (5.6) are also $S_{(1)}$ fractions and have the properties $g_N(0) = 1$, $0 < g_N(x) < 1$, $x \in \mathbb{R}$. The following relations are also satisfied on the positive real axis:

$$w_{2N-2}(x) < \widetilde{w}_{2N}(x) < w_{2N-1}(x),$$
$$w_{2N}(x) < \widetilde{w}_{2N+1}(x) < w_{2N-1}(x). \qquad (5.29)$$

These properties arise from the relation

$$\min\left[\frac{a_1}{b_1}, \frac{a_2}{b_2}\right] < \frac{a_1 + t a_2}{b_1 + t b_2} < \max\left[\frac{a_1}{b_1}, \frac{a_2}{b_2}\right], \quad a_i, b_i > 0, \quad t \geqslant 0, \qquad (5.30)$$

where the following correspondences have been made: $t = c_n z g_n(x)$, $a_1 = A_{n-1}(x)$, $b_1 = B_{n-1}(x)$, $a_2 = A_{n-2}(x)$, $b_2 = B_{n-2}(x)$, and $n = 2N$ or $2N+1$. Uniform convergence of the $w_n(x)$ implies uniform convergence of the $\widetilde{w}_N(x)$ to $f(x)$ on $\mathbb{R}$. By analytic continuation the $\widetilde{w}_N(z)$ converge uniformly to $f(z)$ on compact subsets of $\widetilde{\mathbb{C}}$, and the theorem is proved.

Relation (5.29) actually implies that the uniform convergence of the $\widetilde{w}_N(z)$ to $f(z)$ is guaranteed if the tail of $C(z)$ is replaced by any real positive symmetric function $g_{N-1}(z)$. The exact association of the functions $\widetilde{E}_N(z)$ with the infinite field expansion (5.1) may now be stated.

Theorem 5.2: In the asymptotic expansion of the $\widetilde{E}_N(z)$ in Eq. (5.28), the exponents $\mu(1)$ and $\mu(2)$, which are independent of N, coincide with the leading two powers in the infinite field expansion

$$E(z) - E^{(0)} \sim H_1 z^{\mu(1)} + H_2 z^{\mu(2)}, \quad \text{as } |z| \to \infty,$$

obtained from Eq. (5.1). Moreover, the coefficients $W_1^{(N)}$ and $W_2^{(N)}$ converge uniformly to H_1 and H_2, respectively, as $N \to \infty$.

Proof: This theorem follows from the results of Theorem 5.1 and from the original construction in Eq. (5.27).

Uniform convergence of the approximate convergents $\widetilde{E}_N(z)$ in (5.27) implies that the asymptotic expansion coefficients $W_i^{(N)}, i = 1,2$, converge to the coefficients of the corresponding terms in the infinite field expansion (5.1) as $N \to \infty$.

B. Application to S-fraction representations of the quartic anharmonic oscillator

The goal of this section is to employ the above procedures to recover the leading terms in the infinite field expansion (5.1) for the QAHO,[7] for which $\alpha = \frac{1}{3}$ and $\gamma = \frac{2}{3}$. The coefficients $F_K^{(0)}$ represent the Kth eigenvalues of the quartic oscillator $\hat{H} = \hat{p}^2 + x^4$. We determine the asymptotic expansion of

$$\widetilde{E}_N(z) = E^{(0)} + z\widetilde{w}_N(z), \quad \text{as } z \to \infty, \tag{5.31}$$

where the modified CF, $\widetilde{w}_N(z)$, is constructed as in Sec. V A. It shall always be understood that $z \in \widetilde{C}$.

From Eq. (4.6), we define the relevant parameters

$$k = \tfrac{3}{2}, \quad A^{(1)} = \tfrac{1}{8} + \tfrac{3}{4}K, \quad A^{(2)} = -\tfrac{1}{8} + \tfrac{3}{4}K, \quad \Delta A/k = \tfrac{1}{6}. \tag{5.32}$$

The analysis to follow will be applicable to ground and excited states. The important property $0 < (\Delta A/k) < \frac{1}{2}$, for all states, will be implicitly assumed since it plays a role in the ordering of powers of z, for example, in Eq. (5.17).

For the *odd convergent truncation*, Eqs. (5.10), etc., yield the expansion

$$g_{2n}(z) = D_1^{(2n)} z^{-s} + D_2^{(2n)} z^{-1} + D_3^{(2n)} z^{-2s} + \cdots, \tag{5.33}$$

where $s = \frac{1}{2} + \Delta A/k$ and

$$D_1^{(2n)} = \frac{\Gamma(\frac{1}{2} - \Delta A/k)\Gamma(n + A^{(1)}/k)}{\Gamma(\frac{1}{2} + \Delta A/k)\Gamma(n + \frac{1}{2} + A^{(2)}/k)} \times k^{-(1/2 + \Delta A/k)},$$
$$D_2^{(2n)} = k^{-1}(-\tfrac{1}{2} + \Delta A/k)^{-1}. \tag{5.34}$$

We note that $g_{2n}(z) = O(z^{-2/3})$, as $|z| \to \infty$. Substitution of Eq. (5.33) into (5.17) and multiplication by z yield the formal expansion

$$z\widetilde{w}_{2n-1}(z) \sim W_1^{(2n-1)} z^{1/2 - \Delta A/k} + W_2^{(2n-1)} + \cdots, \tag{5.35}$$

where

$$W_1^{(2n-1)} = \frac{c_{2n-1} D_1^{(2n)} a_{2n-3,n-2}}{b_{2n-2,n-1}},$$
$$W_2^{(2n-1)} = [b_{2n-2,n-1}]^{-1} \times [a_{2n-2,n-2} + c_{2n-1} D_2^{(2n)} a_{2n-3,n-2}]. \tag{5.36}$$

It is immediately noticed that the dominant behavior in Eq. (5.35) is given by $O(z^{1/3})$, in agreement with the infinite field limit.

We now consider the coefficient $W_1^{(2n-1)}$ for a general level of the QAHO, continuing to suppress the index K for notational ease. A look at the closed form expressions in Table I as well as the recursion relations (2.4) reveal that the polynomial coefficients which occur in Eq. (5.36) have the simple form

$$a_{2n-3,n-2} = c_1 c_3 c_5 \cdots c_{2n-3},$$
$$b_{2n-2,n-1} = c_2 c_4 c_6 \cdots c_{2n-2}. \tag{5.37}$$

The leading coefficient in Eq. (5.35) for the Kth level becomes

$$W_1^{(2n-1),K} = \left[\prod_{i=1}^{n-1} \frac{c_{2i-1}^K}{c_{2i}^K}\right] c_{2n-1}^K \times \frac{\Gamma(\frac{1}{3})\Gamma(n + \frac{1}{12} + K/2)}{\Gamma(\frac{2}{3})\Gamma(n - \frac{1}{12} + K/2)} k^{-2/3}. \tag{5.38}$$

From Theorem 5.2, it follows that $W_1^{(2n-1),K} \to F_K^{(0)}$, as $n \to \infty$, where the $F_K^{(0)}$ were defined at the beginning of this section. This behavior is observed numerically and will be discussed at the end of this section.

We now focus on the second term of the expansion in (5.35). For the QAHO, no constant terms are present in the infinite field expansion (5.1). From Theorem 5.2, however, we expect that $W_2^{(2n-1),K} \to -E_K^{(0)} = -(2K+1)$, as $n \to \infty$.

Returning to the *even convergent truncation procedure*, Eqs. (5.10), etc., yield the expansion

$$g_{2n+1}(z) \sim D_1^{(2n+1)} z^{-t} + D_2^{(2n+1)} z^{-2t} + D_3^{(2n+1)} z^{-1} + \cdots, \tag{5.39}$$

where $t = \frac{1}{2} - \Delta A/k$ and

$$D_1^{(2n+1)} = \frac{\Gamma(\frac{1}{2} + \Delta A/k)\Gamma(n + \frac{1}{2} + A^{(2)}/k)}{\Gamma(\frac{1}{2} - \Delta A/k)\Gamma(n + 1 + A^{(1)}/k)} k^{-1/2 + \Delta A/k}, \tag{5.40}$$

$$D_2^{(2n+1)} = \frac{\Gamma(n + A^{(1)}/k)}{(\frac{1}{2} - \Delta A/k)} [D_1^{(2n+1)}]^2.$$

We now substitute the above into Eq. (5.17), where $2n-1$ is replaced by $2n$, etc., and multiply by z to find that

$$z\widetilde{w}_{2n}(z) \sim W_1^{(2n)} z^{1/2 - \Delta A/k} + W_2^{(2n)} + \cdots, \tag{5.41}$$

where

$$W_1^{(2n)} = a_{2n-1,n-1} [c_{2n} D_1^{(2n+1)} b_{2n-2,n-1}]^{-1},$$
$$W_2^{(2n)} = \left[a_{2n-2,n-2} - \frac{a_{2n-1,n-1}(n + A^{(1)}/k)}{c_{2n}(\frac{1}{2} - \Delta A/k)}\right] \times [b_{2n-2,n-1}]^{-1}. \tag{5.42}$$

The exponents in (5.41) agree with those of the odd convergent expansion in Eq. (5.35). Proceeding as before, the leading term coefficient for the Kth level may be simplified to

$$W_1^{(2n),K} = \left[\prod_{i=1}^{n} \frac{c_{2i-1}^K}{c_{2i}^K}\right] \frac{\Gamma(\frac{1}{3})\Gamma(n + \frac{13}{12} + K/2)}{\Gamma(\frac{2}{3})\Gamma(n - \frac{1}{12} + K/2)} k^{1/3}. \tag{5.43}$$

Again, it is expected that $W_1^{(2n)} \to F_K^{(0)}$, as $n \to \infty$. In fact, the common limiting behavior of the two leading term coeffi-

TABLE III. The leading term coefficients $W_1^{(2n-1)}$ and $W_1^{(2n)}$ in Eqs. (5.38) and (5.43), respectively, for odd and even truncation expansion of the ground state ($K=0$) quartic anharmonic oscillator S fraction. These coefficients were calculated from the c_n presented in Table II. The exact asymptotic value corresponds to the ground state energy of the quartic oscillator, accurately calculated in Ref. 36.

n	$W_1^{(2n-1)}$	$W_1^{(2n)}$
1	1.224 047 7874	1.136 615 8026
2	1.184 372 7691	1.128 172 1211
3	1.147 912 1127	1.120 524 8180
4	1.131 702 1008	1.114 333 6496
5	1.121 723 1409	1.109 553 1035
6	1.114 927 2483	1.105 798 2023
7	1.109 924 9553	1.102 752 7649
8	1.106 050 6539	1.100 227 0571
9	1.102 941 5164	1.098 092 4465
10	1.100 377 3017	1.096 258 9783
11	1.098 216 7152	1.094 662 9230
12	1.096 364 8471	1.093 257 8234
13	1.094 755 2164	1.092 008 8703
14	1.093 339 6745	1.090 889 4343
15	1.092 082 4154	1.089 878 7881
16	1.090 956 2079	1.088 960 5397
17	1.089 939 9310	1.088 121 5369
18	1.089 016 9206	1.087 351 0914
19	1.088 173 8319	1.086 640 4182
20	1.087 399 8377	1.085 982 2236
25	1.084 302 1726	1.083 294 1739
30	1.082 061 9832	1.081 298 6219
35	1.080 346 3128	1.079 742 6098
40	1.078 978 6658	1.078 485 8784
45	1.077 855 7235	1.077 443 6524
50	1.076 912 4936	1.076 561 3088
Exact	1.060 362 0905	1.060 362 0905

cients may be seen by examining the ratio

$$\frac{W_1^{(2n)}}{W_1^{(2n-1)}} = \frac{k\Gamma(n+1+A^{(1)}/k)}{c_{2n}\Gamma(n+A^{(1)}/k)}$$

$$= \frac{kn+A^{(1)}}{c_{2n}} \to 1\,, \quad \text{as } n\to\infty\,, \tag{5.44}$$

where the final limit follows from Eq. (5.2).

It is also expected that $W_2^{(2n)} \to -E_K^{(0)}$, as before. Here, a

TABLE IV. The leading term coefficients $W_1^{(N),K}$ in Eqs. (5.38) and (5.43) for odd and even truncation expansion of the QAHO excited states, $K=1$ and 2, calculated from exact S-fraction coefficients c_n^K. The entries denoted "Extrap" are obtained from a Thiele–Padé extrapolation of the numerical values for $n \leqslant 40$. The exact values correspond to the eigenvalues $E_K^{(0)}$ of the first and second excited states of the quartic oscillator, as calculated in Ref. 36.

n	$W_1^{(2n-1),1}$	$W_1^{(2n),1}$	$W_1^{(2n-1),2}$	$W_1^{(2n),2}$
10	4.167 460 1887	4.112 230 5151	9.331 761 4599	8.687 772 5465
15	4.086 243 5971	4.056 467 9529	8.605 787 0279	8.372 579 4890
20	4.041 365 6060	4.022 161 4546	8.192 793 1484	8.110 471 3017
25	4.012 117 4604	3.998 449 3352	8.099 262 4616	8.040 537 0703
30	3.991 198 6065	3.980 844 6770	8.033 011 7261	7.988 468 4132
35	3.975 315 0468	3.967 126 7485	7.983 089 7907	7.947 836 1085
40	3.962 740 8882	3.956 058 0405	7.943 812 7059	7.915 026 9928
Extrap	3.800	3.799 6	7.46	7.456
Exact	3.799 673 0298	3.799 673 0298	7.455 697 9380	7.455 697 9380

ratio analogous to (5.44) exists between coefficients obtained from odd and even truncations.

Numerical results: The values of the leading term coefficients $W_1^{(2n-1)}$ and $W_1^{(2n)}$ in Eqs. (5.38) and (5.43), calculated from the exact coefficients c_n of Table II, are presented in Table III. A regular monotonic behavior toward the exact value[36] $F_0^{(0)} = 1.060\,362\,09...$ is observed for both sequences. For $n = 52$, the coefficients are in error by about 1.5%. The accurate estimation of this constant from LOPT has been a subject of some interest.[13,37] A number of extrapolation techniques were adopted to determine whether these sequences could predict the exact values more accurately.

In one method, the sequence of S-fraction coefficients c_n was artificially extended by a Thiele–Padé CF extrapolation which employed the asymptotics of Eq. (4.6). The approximate coefficients $\hat{c}_n$ were calculated to $n = 18\,000$. Eqs. (5.38) and (5.43) were then evaluated by employing the leading three terms of an asymptotic relation for the ratio of the $\Gamma(n)$ functions. The result was $\widehat{W}_1^{(18\,000)} = 1.061\,550\,0$, which is in error by 0.11%. Needless to say, this method converges very slowly—a 180-fold increase in the number of c_n yields only a tenfold increase in accuracy.

TABLE V. Numerical values of the coefficients $W_2^{(N),K}$ for odd and even convergent expansions of the QAHO, $K=0$ and 1 states, as calculated from exact S-fraction coefficients c_n^K using Eqs. (5.36) and (5.42). The entries denoted "Extrap" are obtained from a Thiele–Padé extrapolation of the numerical values. The exact values correspond to $-E_K^{(0)} = -(2K+1)$, the negatives of the unperturbed harmonic oscillator eigenvalues.

n	$W_2^{(2n-1),0}$	$W_2^{(2n),0}$	$W_2^{(2n-1),1}$	$W_2^{(2n),1}$
10	− 1.319 182 0604	− 1.307 525 7128	− 5.797 418 9494	5.638 473 0622
15	− 1.295 084 5542	− 1.287 925 1310	− 5.562 695 7668	5.464 876 2762
20	− 1.279 587 8618	− 1.274 511 5840	− 5.415 005 9102	5.345 663 1522
25	− 1.268 236 7160	− 1.264 445 2638	− 5.309 333 3028	5.256 213 5888
30	− 1.259 587 9252	− 1.256 454 5210	− 5.228 033 6260	5.185 296 6200
35	− 1.252 476 9026	− 1.249 867 1622	− 5.162 492 9676	5.126 926 9212
40	− 1.246 515 1018	− 1.244 287 2144	− 5.107 904 0762	5.077 564 8328
Extrap	− 1.00 ± 0.02	− 1.00 ± 0.02	− 3.0 ± 0.2	− 2.9 ± 0.2
Exact	− 1	− 1	− 3	− 3

A final attempt to accelerate the slow convergence of this sequence was to Thiele-extrapolate the approximate $\widehat{W}_1^{(N)}$ values of above to their infinite limit. Sets of $[n,n]$ Thiele–Padé approximants were constructed from all sets of $2n+1$ consecutive members of the sequence $\widehat{W}_1^{(N)}$, $N = 1000, 2000, ..., 18\,000$. The common limit of these extrapolations for $n = 3,4,5$, and 6 was 1.060 362 075, a result in error by less than 0.000 000 02. This represents the most accurate calculation of the infinite coupling constant limit from LOPT. The accuracy surpasses the calculations of Refs. 13 and 37.

A similar behavior is observed for the sequences of leading term coefficients for excited state representations. Some values from the sequences corresponding to the levels $K = 1$ and 2 are presented in Table IV. Also given are estimated limits of the sequences as predicted by a Thiele–Padé extrapolation of the elements of these sequences only.

Table V presents some values of the coefficients $W_2^{(N)}$ for both odd and even convergent expansions associated with the ground and first excited states, $K = 0$ and 1, respectively. These values were calculated from the exact S-fraction coefficients. Their convergence to the theoretical values $-E_K^{(0)}$ is not as rapid as for the leading term coefficients. Also presented are Thiele–Padé CF extrapolations of these sequences which are in good agreement with the theoretical values.

C. S-fraction representations of charmonium

The infinite field expansion for the charmonium model has the form of Eq. (5.1) with $\alpha = \frac{2}{3}$ and $\gamma = \frac{1}{3}$. The leading term coefficients $F_{NLM}^{(0)}$ represent eigenvalues of a three-dimensional Airy-type differential equation.[16,30] We now construct a CF representation analogous to Eq. (5.31) and investigate its large field asymptotics.

The asymptotic behavior of the charmonium $S_{(1)}$-fraction coefficients was given in Eq. (4.13). The parameters relevant to the following analysis are

$$
\begin{aligned}
k &= \tfrac{3}{2} N^3 , \\
A^{(1)} &= N^3(-\tfrac{1}{2} + \tfrac{3}{2} N), \\
A^{(2)} &= N^3(-\tfrac{1}{4} + \tfrac{3}{2} N), \\
\Delta A / k &= -\tfrac{1}{6} .
\end{aligned}
\tag{5.45}
$$

We summarize the results of both truncation procedures below.

Odd convergent truncation: Referring to Eq. (5.16), we have $r(1) = -\frac{1}{3}$ and $r(2) = -\frac{2}{3}$ and

$$
\begin{aligned}
D_1^{(2n)} &= \frac{\Gamma(\frac{2}{3})\Gamma(n - \frac{1}{3} + N)}{\Gamma(\frac{1}{3})\Gamma(n + \frac{1}{3} + N)} \left(\frac{2}{3}\right)^{1/3} N^{-1} , \\
D_2^{(2n)} &= 3(n - \tfrac{2}{3} + N)[D_1^{(2n)}]^2 .
\end{aligned}
\tag{5.46}
$$

The net result is

$$
z\widetilde{w}_{2n-1}(z) \sim W_1^{(2n-1)} z^{2/3} + W_2^{(2n-1)} z^{1/3} + \cdots , \tag{5.47}
$$

where

$$
\begin{aligned}
W_1^{(2n-1)} &= \frac{c_{2n-1} D_1^{(2n)} a_{2n-3,n-2}}{b_{2n-2,n-1}} , \\
W_2^{(2n-1)} &= W_1^{(2n-1)} \left[\frac{D_2^{(2n)}}{D_1^{(2n)}} - W_1^{(2n-1)} \frac{b_{2n-3,n-2}}{a_{2n-3,n-2}} \right] .
\end{aligned}
\tag{5.48}
$$

Even convergent truncation: Referring to Eq. (5.22), we have $s(1) = \frac{2}{3}$, $s(2) = 1$, and

$$
\begin{aligned}
D_1^{(2n+1)} &= \frac{\Gamma(\frac{1}{3})\Gamma(n + \frac{1}{3} + N)}{\Gamma(\frac{2}{3})\Gamma(n + \frac{2}{3} + N)} (\tfrac{2}{3})^{2/3} N^{-2/3} , \\
D_2^{(2n+1)} &= -3/k .
\end{aligned}
\tag{5.49}
$$

The net result is

$$
z\widetilde{w}_{2n}(z) \sim W_1^{(2n)} z^{2/3} + W_2^{(2n)} z^{1/3} + \cdots , \tag{5.50}
$$

where

$$
\begin{aligned}
W_1^{(2n)} &= \frac{a_{2n-1,n-1}}{c_{2n} D_1^{(2n+1)} b_{2n-2,n-1}} , \\
W_2^{(2n)} &= W_1^{(2n)} \left[-\frac{D_2^{(2n+1)}}{D_1^{(2n+1)}} - W_1^{(2n)} \frac{b_{2n-1,n-1}}{a_{2n-1,n-1}} \right] .
\end{aligned}
\tag{5.51}
$$

We immediately notice that the leading exponent $\alpha = \frac{2}{3}$ is obtained from the term $\frac{1}{2} - \Delta A / k$. The leading term coefficients $W_1^{(2n-1)}$ and $W_2^{(2n)}$ have the same generic form as their QAHO counterparts in Eqs. (5.38) and (5.43). For a general

TABLE VI. Numerical values of the leading term coefficients $W_1^{(k)}$ in Eqs. (5.52) and (5.53) for truncations of the ground state charmonium S fraction. The exact value is the ground state of an Airy differential equation.

n	$W_1^{(2n-1)}$	$W_1^{(2n)}$
1	0.502 195 6152	1.255 489 0381
2	1.255 489 0381	1.365 191 9638
3	1.397 286 2825	1.452 522 4410
4	1.468 149 2263	1.506 058 7769
5	1.515 535 3965	1.543 038 1825
6	1.549 352 0460	1.570 587 0907
7	1.575 100 4133	1.592 108 1965
8	1.595 479 8492	1.609 502 3004
9	1.612 117 7745	1.623 936 6885
10	1.626 021 2941	1.636 157 5755
11	1.637 856 5953	1.646 674 8240
12	1.648 085 4000	1.655 848 0979
13	1.657 037 1400	1.663 938 9765
14	1.664 954 3381	1.671 143 2758
15	1.672 020 0523	1.677 610 7481
16	1.678 375 1994	1.683 458 0510
17	1.684 130 2254	1.688 777 6125
18	1.689 373 0844	1.693 643 7351
19	1.694 174 7790	1.698 116 9063
20	1.698 593 3221	1.702 246 9261
25	1.716 369 0297	1.718 992 1717
30	1.729 305 5925	1.731 305 1658
35	1.739 252 2482	1.740 841 1185
40	1.747 201 9267	1.748 503 5446
45	1.753 740 9885	1.754 332 4751
50	1.759 240 6071	1.760 172 9309
Exact	1.855 757 081	1.855 757 081

TABLE VII. Results of a Thiele–Padé estimation of the limits of leading term coefficients $W_1^{(k)}$ in Eqs. (5.52) and (5.53), as $k\rightarrow\infty$, k even and odd, for the six lowest-lying charmonium states. The limits $W_1^{(\infty)}$ are presented to the number of digits shared by estimates for even-k and odd-k sequences. The exact values $F_{NL}^{(0)}$, which correspond to the (N,L) state eigenvalues of a three-dimensional Airy differential equation, are taken from Ref. 30.

State	N	L	$W_1^{(\infty)}$	$F_{NL}^{(0)}$
1S	1	0	1.855 75	1.855 757
2S	2	0	3.24	3.244 6
2P	2	1	2.668	2.667 9
3S	3	0	4.4	4.381 7
3P	3	1	3.9	3.876 8
3D	3	2	3.37	3.371 8

state $|N,L,M\rangle$, they assume the explicit form

$$W_1^{(2n-1),NLM}=\left[\prod_{i=1}^{n-1}\frac{c_{2i-1}^{NLM}}{c_{2i}^{NLM}}\right]c_{2n-1}^{NLM}\times\frac{\Gamma(\frac{2}{3})\Gamma(n-\frac{1}{3}+N)}{N\Gamma(\frac{1}{3})\Gamma(n+\frac{1}{3}+N)}\left(\frac{2}{3}\right)^{1/3}, \tag{5.52}$$

$$W_1^{(2n),NLM}=\left[\prod_{i=1}^{n}\frac{c_{2i-1}^{NLM}}{c_{2i}^{NLM}}\right]\frac{\Gamma(\frac{2}{3})\Gamma(n+\frac{2}{3}+N)}{\Gamma(\frac{1}{3})\Gamma(n+\frac{1}{3}+N)}N^2\left(\frac{3}{2}\right)^{2/3}. \tag{5.53}$$

An analysis of the same form as in Eq. (5.44) reveals that the above constants approach a common limit as $n\rightarrow\infty$. From Eq. (5.1), it is expected that this common limit is $F_{NLM}^{(0)}$.

Numerical results: The values of the leading term coefficients $W_1^{(2n-1)}$ and $W_2^{(2n)}$ in Eq. (5.52), corresponding to the ground state $N=1$, $L=M=0$, are presented in Table VI. A regular monotone behavior approaching the exact value $F^{(0)}=1.855\,757\,081$ is observed for both sequences. A Thiele–Padé extrapolation of values from each sequence affords approximate limits which are in excellent agreement with the exact results. Table VII presents the results of these extrapolations for all states $1<N<3$, $L=0,1,2,\ldots,N$. The estimates are presented to the number of digits shared by extrapolations of even and odd sequences. In all cases, the estimated limits are in good agreement with the exact values taken from Ref. 30.

TABLE VIII. Numerical values of the second term coefficients $W_2^{(k)}$ in Eqs. (5.48) and (5.51) for ground state charmonium, as obtained from exact S-fraction coefficients c_n^{100}. The entries denoted "Extrap" are obtained from Thiele extrapolation of the sets of numerical values. They represent estimates of the expectation value of the negative Coulomb potential over the unperturbed ground state Airy function.

n	$W_2^{(2n-1)}$	$W_2^{(2n)}$
10	0.727 593 170 3	0.706 640 967 7
15	0.623 259 099 7	0.608 708 767 3
20	0.549 905 928 8	0.538 892 017 4
25	0.493 981 747 5	0.485 182 577 5
30	0.449 114 911 4	0.441 823 389 1
35	0.411 841 069 4	0.405 637 637 0
40	0.380 080 166 3	0.374 696 598 4
Extrap	-0.26 ± 0.02	-0.26 ± 0.03

Table VIII presents some values of the coefficients $W_2^{(2n-1)}$ and $W_2^{(2n)}$ corresponding to the ground state, along with the Thiele–Padé extrapolated limits of both sequences. Interestingly, the limits of these positive and monotone decreasing sequences are negative, which is to be expected, since they correspond to the expectation value of a negative Coloumb potential over the unperturbed Airy eigenfunctions.

VI. THE RELATION BETWEEN SUBDOMINANT TERMS IN LOPT AND CFLO FOR $S_{(1)}$ FRACTIONS

Here we show, by example, that a simple relationship does not exist between $n!$-type Stieltjes series coefficients and their $S_{(1)}$-fraction counterparts as far as subdominant terms are concerned. We shall refer to the relevant expansions for the quartic anharmonic oscillator, Eqs. (4.4) and (4.6), and inquire whether a relationship exists between the $1/n$ correction term in Eq. (4.4) and the constant terms in Eq. (4.6). The knowledge of these terms in closed form serves as a motivation. The following treatment will be centered around the QAHO problem, and special reference to the charmonium model will be made at the end.

For convenience, we consider the following scaled QAHO perturbation coefficients,

$$E_K^{(n)}=(-1)^{n+1}\Gamma(n+K+\tfrac{1}{2})[1+A_Kn^{-1}+O(n^{-2})], \tag{6.1}$$

where

$$A_K=-(\tfrac{95}{72}+\tfrac{29}{12}K+\tfrac{17}{12}K^2) \tag{6.2}$$

and the geometric factor $k=\frac{3}{2}$ is combined with the coupling constant β to produce the expansion parameter $z=k\beta$. The multiplicative factor has also been ignored as it will only contribute to c_1^K. The coefficients of the $S_{(1)}$ fraction which represents the scaled series beginning with term $E_K^{(1)}$ are given by

$$c_n^K=n/2+K/2\pm\tfrac{1}{12}+R_n^{(i),K},\quad n\geq2,\quad i=\begin{cases}1, & n\ \text{even},\\ 2, & n\ \text{odd},\end{cases} \tag{6.3}$$

where it has been conjectured that $R_n^{(i),K}=O(n^{-1/2})$. Let us now consider the "model" perturbation series whose coefficients contain only the dominant terms of the $E_K^{(n)}$ in (4.1), i.e.,

$$\overline{E}(z)=1+\sum_{n=1}^{\infty}\overline{E}_K^{(n)}z^n=1+\sum_{n=1}^{\infty}(-1)^{n+1}\Gamma\left(n+K+\frac{1}{2}\right)z^n. \tag{6.4}$$

From Eq. (3.11), the coefficients of the S-fraction representation, $\overline{E}(z)=1+z\overline{C}(z)$, are given by

$$\bar{c}_1^K=\Gamma(K+\tfrac{3}{2}),\quad \bar{c}_{n,\text{even}}^K=n/2+K+\tfrac{1}{2},\quad \bar{c}_{n,\text{odd}}^K=n/2-\tfrac{1}{2}. \tag{6.5}$$

A comparison between Eqs. (6.3) and (6.5) gives the interesting set of relations,

$$c_n^K = \bar{c}_n^K + (-1)^{n+1}\epsilon^K + R_n^{(i),K} = d_n^K + R_n^{(i),K}, \quad n \geq 2, \tag{6.6}$$

where

$$\epsilon^K = K/2 + \tfrac{5}{12}. \tag{6.7}$$

In other words, the "true" QAHO coefficients c_n are obtained by perturbing the model hypergeometric $\bar{c}_n^K$ with a constant term alternating in sign and correction terms of order $o(1)$. One may well ask whether the oscillating perturbation alone could account for the appearance of the term A_K/n in (6.1), which, in turn, arises from a transformation of the series in (6.4). In other words, given the formal CF-power series correspondence,

$$\mathop{\mathrm{K}}_{n=1}^{\infty} \frac{d_n^K z}{1} = \sum_{n=1}^{\infty} (-1)^{n+1}\Gamma\left(n + K + \frac{1}{2}\right) \times\left(1 + \frac{B_K}{n} + \cdots\right)z^n, \tag{6.8}$$

does $B_K = A_K$?

In order to answer this question, we define

$$F(z,\epsilon) = 1 + z\Gamma(a-\epsilon)\Gamma(1+\epsilon)\,\frac{{}_2F_0(a-\epsilon,1+\epsilon,-z)}{{}_2F_0(a-\epsilon,\epsilon,-z)}, \tag{6.9}$$

where $a = K + \frac{3}{2}$ so that $F(z,0) = \overline{E}(z)$. For ease of notation, the index K will be supressed in the following presentation. From Eq. (5.8), the function $F(z,\epsilon)$ is seen to admit the S-fraction representation

$$F(z,\epsilon) = 1 + \mathop{\mathrm{K}}_{n=1}^{\infty} \frac{\bar{c}_n^K + (-1)^{n+1}\epsilon}{1}. \tag{6.10}$$

We now expand $F(z,\epsilon)$ as a power series in z,

$$F(z,\epsilon) = 1 + \sum_{n=1}^{\infty} F^{(n)} z^n, \tag{6.11}$$

and seek to express the coefficients $F^{(n)}$ as

$$F^{(n)} \sim (-1)^{n+1}\Gamma(n + a - 1)[1 + B/n + \cdots], \tag{6.12}$$

where B will be determined in terms of a and ϵ. We let

$${}_2F_0(a-\epsilon, 1+\epsilon; -z) = \sum_{n=0}^{\infty} a_n z^n, \tag{6.13}$$

$${}_2F_0(a-\epsilon,\epsilon;-z) = \sum_{n=0}^{\infty} b_n z^n \tag{6.14}$$

$$= \left[\sum_{n=0}^{\infty} p_n z^n\right]^{-1}. \tag{6.15}$$

The general coefficient $F^{(n)}$ in Eq. (6.11) will have the formal Cauchy composition

$$F^{(n)} = \Gamma(a-\epsilon)\Gamma(1+\epsilon)(a_0 p_{n-1} + a_1 p_{n-2} + \cdots + a_{n-2}p_1 + a_{n-1}p_0). \tag{6.16}$$

Formal expansion of the hypergeometric function in Eq. (6.13) and use of the relation[38]

$$\Gamma(n+r) \sim \Gamma(n+s)n^{r-s}[1 + (r-s)(r+s-1)/(2n) + O(n^{-2})], \quad \text{as } n \to \infty, \tag{6.17}$$

yields

$$a_{n-1} = (-1)^{n-1}\Gamma(n+a-1)/\Gamma(a-\epsilon)\Gamma(1+\epsilon) \times [1 + (\epsilon^2 - (a-1)\epsilon)/n + O(n^{-2})]. \tag{6.18}$$

Furthermore, $c_0 = 1$, so we have determined the contribution from $p_0 a_{n-1}$ in (6.16). In order to find the contribution from $a_{n-2}p_1$, we use the fact that $p_1 = \epsilon(a-\epsilon)$ and apply relation (6.17) to (6.13) to obtain

$$a_{n-2}p_1 = (-1)^n\Gamma(n+a-1)/(\Gamma(a-\epsilon)\Gamma(1+\epsilon)) \times [(a-\epsilon)\epsilon/n + O(n^{-2})]. \tag{6.19}$$

The term $a_{n-3}p_2$ contributes terms of order $O(n^{-2})$ to (6.16) and, along with lower terms, need not be considered, with the exception of the final term $a_0 p_n$.

To determine the asymptotic behavior of the coefficients p_n of the inverse series in Eq. (6.15), we employ the method discussed by Bender.[39] It is sufficient to show that if (i) $b_n \neq 0$, $b_{n-1} = o(b_n)$, and (ii) there exists an $R > 0$ such that for n sufficiently large

$$S_R \equiv \sum_{k=R}^{n-R} |b_k b_{n-k}| = O(b_{n-R}),$$

then the coefficients p_n are given by

$$p_n = \sum_{k=0}^{R-1} g_k b_{n-k} + O(b_{n-R}),$$

where the g_k are coefficients of the power series expansion

$$-\left[\sum_{n=0}^{\infty} b_n z^n\right]^{-2} = \sum_{n=0}^{\infty} g_n z^n.$$

The above properties are easily established from the exact form of the b_n coefficients and the final result is

$$p_n = \frac{(-1)^{n+1}}{\Gamma(a-\epsilon)\Gamma(\epsilon)}\Gamma(n+a)\left[\frac{1}{n} + O(n^{-2})\right]. \tag{6.20}$$

The net contribution from Eqs. (6.18), (6.19), and (6.20) to Eq. (6.16) is

$$B_K = 2\epsilon^2 - 2a\epsilon. \tag{6.21}$$

For the quartic anharmonic oscillator, $\epsilon = K/2 + \frac{5}{12}$ and $a = K + \frac{3}{2}$, so that

$$B_K = -(\tfrac{65}{72} + \tfrac{3}{2}K + \tfrac{1}{2}K^2). \tag{6.22}$$

Numerical results for $K = 0, 1, 2, 3$, and 4 are in exact agreement with this expression. Clearly, this term does not equal the true asymptotic correction for the QAHO perturbation coefficients in (6.2).

Turning to the $L = 0$ charmonium representations, we consider the scaled series coefficients

$$E_N^{(n)} = (-1)^{n+1}\Gamma(n+2N) \times [1 - \tfrac{1}{9}(10 + 18N + 21N^2)(1/n) + O(n^{-2})]. \tag{6.23}$$

The expansion parameter becomes $z = \frac{3}{2}N^3\lambda$. The associated S-fraction coefficients have the form

$$c_n^N = \frac{n}{2} + \begin{cases} N - \frac{1}{3} \\ N - \frac{1}{6} \end{cases} + R_n^{(i),N}, \quad \begin{cases} n \text{ even}, \\ n \text{ odd}. \end{cases} \tag{6.24}$$

The relevant parameters in Eq. (6.21) are $a = 2N + 1$ and $\epsilon = N + \frac{1}{3}$. Thus, we have

$$B_N = -(\tfrac{4}{9} + 2N + 2N^2), \tag{6.25}$$

again in disagreement with the LOPT result in (6.23).

This represents the limit of any closed-form analysis. Numerical experiments suggest that all subdominant terms in $R_n^{(i)}$ contribute to the $1/n$ correction to the perturbation series. The experiments and mechanism will be discussed elsewhere.

ACKNOWLEDGMENTS

We express our sincere thanks to Professor J. Paldus for helpful discussions throughout the course of this work.

This work was supported in part by a Natural Sciences and Engineering Research Council (NSERC) of Canada Grant in Aid of Research (J.C.) as well as an NSERC Postgraduate Scholarship and a Province of Ontario Queen Elizabeth II Scholarship (E.R.V.), which are hereby gratefully acknowledged.

APPENDIX: PROOF OF PROPOSITION 3.1

In this section we prove Proposition 3.1 [c.f. Eq. (3.7)]: Given a Stieltjes series $f(z)$ whose coefficients behave asymptotically as

$$a_n \sim (-1)^{n+1}\Gamma(n+a)k^n(1+A/n+\cdots), \quad \text{as } n\to\infty, \tag{A1}$$

where a, k, and A are real constants, then the coefficients of its S-fraction representation $f(z)=a_0+zC(z)$ behave asymptotically as

$$c_n \sim \tfrac{1}{2}kn, \quad \text{as } n\to\infty. \tag{A2}$$

We now consider this quotient-difference (QD) table for the above series, as defined by Eqs. (2.11) and (2.12) and illustrated in Fig. 1. The existence and uniqueness of the QD table, hence the c_n, is guaranteed from the hypothesis that $f(z)$ is Stieltjes. From Eq. (2.11) it follows that the elements of the column q_{n1} behave asymptotically as

$$q_{n1}=k(n+a)+O(n^{-1}), \quad \text{as } n\to\infty. \tag{A3}$$

The following expansions are now assumed for the columns,

$$\begin{aligned} q_{nm} &= n[B_{0m}+B_{1m}/n+B_{2m}/n^2+\cdots], \\ &\quad m=1,2,\ldots, \quad \text{as } n\to\infty, \\ e_{nm} &= C_{0m}+C_{1m}/n+C_{2m}/n^2+\cdots, \\ &\quad m=1,2,\ldots, \quad \text{as } n\to\infty. \end{aligned} \tag{A4}$$

From Eq. (A3), we have $B_{0m}=k$.

Substitution of the above expansions into the rhombus rules, Eq. (2.12) shows that the first four expansion coefficients are given by

$$\begin{aligned} C_{0m} &= mB_{01}, & B_{0m} &= B_{0,m-1}=\cdots=B_{01}, \\ C_{1m} &= 0, & B_{1m} &= B_{1,m-1}=\cdots=B_{11}, \\ C_{2m} &= -mB_{21}, & B_{2m} &= B_{2,m-1}=\cdots=B_{21}, \\ C_{3m} &= -2m^2-m(2B_{31}+B_{21}), & B_{3m} &= B_{30}+2mB_{21}. \end{aligned} \tag{A5}$$

In other words, the elements of the q_{nm} columns are growing linearly downward as $B_{01}n$, while those of the e_{nm} columns approach the constants C_{0m}. However, these constants $C_{0m}=mB_{01}$ grow linearly as we move outward horizontally.

e_{00}		e_{01}		e_{02}		e_{03}		e_{04}
	q_{11}		q_{12}		q_{13}		q_{14}	
e_{10}		e_{11}		e_{12}		e_{13}		
	q_{21}		q_{22}		q_{23}			
e_{20}		e_{21}		e_{22}				
	q_{31}		q_{32}					
e_{30}		e_{31}						
	q_{41}							

FIG. 2. The *extended* QD table associated with the QD table presented in Fig. 1. The upper triangle array represents the quotient-difference array for the inverse power series. The rows e_{0m} and q_{1m} are initialized according to Eqs. (A6). The rhombus rules in Eq. (A8) permit a downward calculation of the array from these rows to the diagonal elements q_{nn} and e_{nn}. This constitutes the *extended QD scheme*.

We now consider an extension[23] of the QD array of Fig. 1 to produce a rectangular array as shown in Fig. 2. All elements obey the rhombus rules as before. The elements of the first two rows of the extended array are given by

$$\begin{aligned} q_{11} &= -a_1/a_0=b_1/b_0, \\ q_{1m} &= 0, \quad m=2,3,4,\ldots, \\ e_{1m} &= -b_{m+1}/b_m, \quad m=2,3,4,\ldots, \end{aligned} \tag{A6}$$

where the b_i are coefficients of the reciprocal power series,

$$[a_0+a_1z+a_2z^2+\cdots]^{-1}=b_0+b_1z+b_2z^2+\cdots. \tag{A7}$$

All elements of the QD array in Fig. 2 may, in fact, be calculated from the initial values in Eq. (A6) by rearranging the rhombus rules as follows:

$$\begin{aligned} e_{nm} &= e_{n-1,m}q_{n,m+1}/q_{nm}, \\ q_{nm} &= q_{n-1,m}+e_{n-1,m}-e_{n-1,m-1}, \\ &\quad m=2,3,\ldots, \quad n=2,3,\ldots. \end{aligned} \tag{A8}$$

This method of calculating the QD array is known as the *extended QD scheme.*

From the asymptotic analysis of reciprocal series described in Ref. 39 and outlined in Sec. VI, it follows that the coefficients b_i of the inverse power series in (A6) behave asymptotically as

$$b_n \sim (-1)^n\Gamma(n+a)k^n(1+B/n+\cdots), \quad \text{as } n\to\infty. \tag{A9}$$

It follows that the elements of the first nonzero row e_{1m} behave asymptotically as

$$e_{1m}\sim k(n+a)+O(n^{-1}), \quad \text{as } n\to\infty. \tag{A10}$$

We now consider row-wise asymptotic expansions, analogous to (A4), and having the form

$$\begin{aligned} e_{nm} &= m[\widetilde{B}_{n0}+\widetilde{B}_{n1}/m+\widetilde{B}_{n2}/m^2+\cdots], \quad \text{as } m\to\infty, \\ q_{nm} &= \widetilde{C}_{n0}+\widetilde{C}_{n1}/m+\widetilde{C}_{n2}/m^2+\cdots, \quad \text{as } m\to\infty. \end{aligned} \tag{A11}$$

These expansions exploit the fundamental symmetry property of the extended QD scheme: q-columns behave as e-rows, and e-columns behave as q-rows. The following relations between expansion coefficients also reflect this property:

$$\begin{aligned} \widetilde{C}_{n0} &= n\widetilde{B}_{10}, & \widetilde{B}_{n0} &= \widetilde{B}_{n-1,0} = \cdots = \widetilde{B}_{10}, \\ \widetilde{C}_{n1} &= 0, & \widetilde{B}_{n1} &= \widetilde{B}_{n-1,1} = \cdots = \widetilde{B}_{11}, \\ \widetilde{C}_{n2} &= -n\widetilde{B}_{12}, & \widetilde{B}_{n2} &= \widetilde{B}_{n-1,2} = \cdots = \widetilde{B}_{12}, \\ \widetilde{C}_{n3} &= -2n^2 - n(2\widetilde{B}_{12} + \widetilde{B}_{02}), & \widetilde{B}_{n3} &= \widetilde{B}_{03} + 2n\widetilde{B}_{12}. \end{aligned} \tag{A12}$$

Thus, for the upper triangular section of the extended QD scheme, the e_{nm} rows grow outward linearly as $\widetilde{B}_{10}m$ while the q_{nm} rows approach constants $\widetilde{C}_{n0}$. However, these constants grow linearly as $\widetilde{B}_{10}n$ as we move downward.

The growth rates for rows and columns of upper and lower triangles of the extended QD array are now seen to match, implying that the diagonal elements grow as $q_{nn} = B_{01}n$, $e_{nn} = B_{01}n$. Since $B_{01} = k$ and $c_{2n} = q_{nn}$, $c_{2n+1} = e_{nn}$, it follows that $c_n \sim kn/2$.

The condition that the a_n have an asymptotic expansion in powers of $1/n$ in Eq. (A1) is evidently strong but not necessary. We have relied on the observation that many of the typical perturbation coefficients encountered in quantum mechanics possess such expansions. This enables us to assume the expansions in (A4) and (A11).

Before closing this section, let us make one final remark concerning the application of the above analysis to other $S_{(k)}$ fractions. For $S_{(2)}$ fractions, the expansions analogous to (A4) and (A7) involve quadratic growth of the q-columns and linear growth of the e-columns. There is a net quadratic growth of entries both horizontally and vertically but the elucidation of the constant coefficient from the relations analogous to Eqs. (A5) and (A12) is much more complicated. Unlike in the $S_{(1)}$ case, all terms B_{nm} and C_{nm} contribute to this constant. This feature will be discussed in a future report.

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