Algebraic methods, Bender-Wu formulas, and continued fractions at large order for charmonium

E. R. Vrscay*
Quantum Theory Group, Department of Applied Mathematics, Faculty of Mathematics, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1
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A special coordinate realization of the Lie algebra so(4,2) is used to reformulate the perturbation problem of a hydrogen atom in a linear radial potential over a complete and discrete Sturmian basis. In this way, the Rayleigh-Schrödinger coefficients $E_{NLM}^{(n)}$ may be calculated to arbitrarily high order for any state. The large-order behavior of these coefficients is determined by Bender-Wu WKB theory. A general formula for the large-order behavior of the coefficients c_n^{NLM} of the Stieltjes continued-fraction representations of these perturbation expansions is given and related to that of the $E_{NLM}^{(n)}$.

I. INTRODUCTION

The model problem of a hydrogenic atom in a linear radial potential—the charmonium model—is given by the Hamiltonian (in atomic units)

$$\hat{H}(\lambda)=-\tfrac{1}{2}\nabla^2-\frac{Z}{r}+\lambda r\ . \tag{1.1}$$

It has attracted great interest in both the areas of quantum chromodynamics (QCD) and atomic and molecular physics (AMP). Regarding the former, the spectra of families of elementary particles may be well described by bound states of charmed-quark—charmed-antiquark pairs interacting through various nonrelativistic confinement potentials.[1,2] Equation (1.1) is a specific example of a wide class of Hamiltonians which have been studied in this context.[3]

Of relevance to AMP, Eq. (1.1) is, for $Z=1$, the spherically symmetric analog of the Stark effect in hydrogen. For $\lambda<0$, corresponding to an unstable potential, $E(\lambda)$ is complex and $-\mathrm{Im}E$ is inversely proportional to the mean lifetime of the exponentially decaying tunneling states or resonances.[4] For this reason, Titchmarsh[5] studied the asymptotics of $\mathrm{Im}E$ as $\lambda\to 0$ as a natural precursor to the study of resonances in the Stark effect and the famous Oppenheimer formula (and its variations). In their detailed analysis of resonances, Harrell and Simon[6] continued this theme and determined the asymptotics of $\mathrm{Im}E$ in (1.1) using the techniques of ordinary differential equations in the complex plane. Regarding (1.1) as a screened Coulomb potential problem, Mehta and Patil[7] employed Bender-Wu WKB methods to determine these asymptotics for spherically symmetric (zero angular momentum) states. The large-order behavior of the Rayleigh-Schrödinger perturbation coefficients for these states was determined with the use of dispersion relations.

Traditional perturbation and variation treatments of hydrogenic perturbation problems such as Eq. (1.1) are hampered by the presence of the continuum states of the unperturbed hydrogen atom. Various methods which circumvent this difficulty have been devised to calculate Rayleigh-Schrödinger perturbation expansions. Some of these have been applied to Eq. (1.1), for example, the Hellmann-Feynman and hypervirial theorems,[8,9] and a method of quadratures.[10] The Padé-approximant summability of the ground-state perturbation series has also been numerically demonstrated.[8,9]

This report is concerned with Rayleigh-Schrödinger perturbation theory (RSPT) at large order for the Hamiltonian in (1.1). In the spirit of early investigations of divergent perturbation series encountered in nonrelativistic quantum mechanics,[11] and subsequent research,[12,13] the paper involves an interaction of three basic themes which account for its title: (a) the practical calculation of the Rayleigh-Schrödinger (RS) perturbation series for a given energy level; (b) the large-order behavior of the series coefficients, which is important in establishing the summability of the series; and (c) a continued-fraction (CF) representation of this series which, in some respects, may be considered a more natural representation of $E(\lambda)$ than the perturbation series itself.

As the previous paragraphs suggest, various aspects of the RSPT of (1.1) have been studied in the literature. The three themes given above provide a unified treatment of the summability problem for this model, from practice to theory. A little elaboration on these aspects, and how they are to be presented in this paper, now follows.

(a) *Algebraic methods.* In Sec. II we outline the use of a special coordinate realization of the Lie algebra so(4,2) to calculate the RS perturbation expansion for the energy of a given level,

$$E_{NLM}(\lambda)=-\frac{Z^2}{2N^2}+\sum_{n=1}^{\infty}E_{NLM}^{(n)}\lambda^n\ . \tag{1.2}$$

Here, N, L, and M denote, respectively, the principal, orbital-angular-momentum, and magnetic quantum numbers of the unperturbed state which gives rise to the level. (Quantum numbers for a reference state will generally be capitalized to avoid any confusion with lower-case dummy indices.) The coefficients $E_{NLM}^{(n)}$ (which are M independent) are calculated to large order, typically $n\sim 100$.

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In Appendix A, we outline a difference-equation approach which may also be used to calculate the $E_{NLM}^{(n)}$.

(b) *Bender-Wu formulas.* In Sec. III the large-order behavior of the RS coefficients $E_{NLM}^{(n)}$ for general levels is determined by (nonrigorous) WKB methods. Elliptic integrals are used to determine the asymptotics of the tunneling factor integral. The formulas are checked numerically for a number of cases. The high-field limit of charmonium, relevant to this section, is discussed in Appendix B.

(c) *Continued fractions at large order.* Section IV deals with a continued-fraction representation of the series in (1.2) which assumes the form

$$E_{NLM}(\lambda)=-\frac{1}{2N^2}+\lambda C^{NLM}(\lambda)$$
$$=-\frac{1}{2N^2}+\cfrac{c_1^{NLM}\lambda}{1+\cfrac{c_2^{NLM}\lambda}{1+\cfrac{c_3^{NLM}\lambda}{1+\cdots}}}\ . \tag{1.3}$$

The coefficients c_n^{NLM} are calculated accurately to large order ($n\sim 100$) for a number of levels using multiple-precision arithmetic. The large-order behavior of these coefficients is related to that of the $E_{NLM}^{(n)}$, which is confirmed numerically. Some important aspects of RITZ (rotation-inversion-translation-z) fractions are given in Appendix C.

II. THE LIE ALGEBRAS so(4,2) AND so(2,1) AND HYDROGENIC PERTURBATION THEORY

The bound-state (discrete) hydrogenic eigenfunctions are given by

$$\psi_{nlm}(\mathbf{r})=\frac{2}{n^2}\left[\frac{Z^3(n-l-1)!}{(n+l)!}\right]^{1/2}e^{-Zr/n}\left[\frac{2Zr}{n}\right]^l$$
$$\times L_{n-l-1}^{2l+1}(2Zr/n)Y_{lm}(\theta,\phi)\ , \tag{2.1}$$

where n, l, and m are the usual hydrogen quantum numbers,

$$L_k^{\alpha}(x)=\frac{\Gamma(k+\alpha+1)}{\Gamma(k+1)\Gamma(\alpha+1)}\,{}_1F_1(-k;\alpha+1;x) \tag{2.2}$$

denotes the associated Laguerre function, and $Y_{lm}(\theta,\phi)$ represents the spherical harmonics. It is well known that the ψ_{nlm} form an orthonormal system in the Hilbert space $L^2(\mathbb{R}^3)$ which is not complete, due to the simultaneous presence of continuum eigenstates.[14] This represents a great nuisance to any proper perturbation or variational treatment formulated in this basis, since such calculations would necessarily involve summations over discrete states along with integration over the continuum. The latter procedure is tedious and computationally difficult. Many calculations in the literature have ignored this contribution at the expense of accruing a non-negligible loss of accuracy.

The problems associated with the continuum are effectively bypassed when the Schrödinger equation is transformed and reformulated in terms of the elements of a particular coordinate realization of the Lie algebra so(4,2).[15–18] This realization contains several quantum-mechanical operators relevant to the hydrogen atom, including the angular momentum and (modified) Laplace-Runge-Lenz vectors. One advantage of this procedure is that the matrix elements of the algebraic operators are known from representation theory and no integrals need be calculated. In addition, the basis functions χ_{nlm} which span a unitary irreducible representation of this algebra exist in a one-to-one correspondence with the discrete hydrogenic functions ψ_{nlm} but form a complete basis, an ideal situation for perturbation theory. The algebraic method is versatile and has been applied effectively to treat a variety of hydrogenic perturbation problems.[19–23]

We now outline the major features involved in the Lie algebraic reformulation of Eq. (1.1), and then develop the relevant perturbation theory. The spherical symmetry (unidimensionality) of this problem simplifies not only RSPT but also the algebraic treatment, since only the three elements of the Lie subalgebra so(2,1) [the generators of the Lie group SO(2,1) associated with the hydrogen radial equation] are actually required. For more detailed expositions of this method, the reader is referred to Refs. 11 and 18.

The algebraic reformulation of hydrogenic reference problems rests on the selection of an unperturbed reference state. Therefore, for the remainder of this section, it will be understood that we are considering the perturbation of a particular hydrogenic state $\psi_{NLM}\rightarrow\psi_{NLM}(\lambda)$, as described by the eigenvalue equation

$$\left[-\tfrac{1}{2}\nabla^2-\frac{Z}{r}-\lambda r-E_{NLM}(\lambda)\right]\psi_{NLM}(\lambda)=0\ . \tag{2.3}$$

First, define

$$E(\lambda)=-\frac{Z^2}{2N^2}+\Delta E(\lambda) \tag{2.4}$$

(subscripts understood), and rewrite Eq. (2.3) as

$$\left[\tfrac{1}{2}\hat{p}_r^{\,2}+\frac{L(L+1)}{2r^2}+\frac{Z^2}{2N^2}-\frac{Z}{r}+\lambda r-\Delta E\right]\psi=0\ , \tag{2.5}$$

where

$$\hat{p}_r=-\frac{i}{r}\left[\frac{\partial}{\partial r}r\right]$$

is the radial momentum operator. Now apply the transformation[24]

$$r=(Z/N)r'\ ,\quad \hat{p}=(N/Z)\hat{p}'\ , \tag{2.6}$$

to Eq. (2.5), drop the primes, and multiply the resulting equation by r to give

$$\left[\tfrac{1}{2}r\hat{p}_r^{\,2}+\frac{L(L+1)}{2r^2}\right.$$
$$\left.+\tfrac{1}{2}r-N+\lambda\left[\frac{N}{Z}\right]^3r^2-\left[\frac{N}{Z}\right]^2\Delta E\,r\right]\psi=0\ . \tag{2.7}$$

We now define the operators

$$\hat{T}_1=\frac{1}{2}\left[r\hat{p}_r^2+\frac{L(L+1)}{r}-r\right],$$
$$\hat{T}_2=r\hat{p}_r\ , \tag{2.8}$$
$$\hat{T}_3=\frac{1}{2}\left[r\hat{p}_r^2+\frac{L(L+1)}{r}+r\right],$$

which satisfy the commutation relations of an so(2,1) Lie algebra, i.e.,

$$[\hat{T}_1,\hat{T}_2]=-i\hat{T}_3\ ,$$
$$[\hat{T}_2,\hat{T}_3]=i\hat{T}_1\ , \tag{2.9}$$
$$[\hat{T}_3,\hat{T}_1]=i\hat{T}_2\ ,$$

where $[\hat{A},\hat{B}]\equiv\hat{A}\hat{B}-\hat{B}\hat{A}$. Since $r=\hat{T}_3-\hat{T}_1$, the eigenvalue equation (2.7) may be expressed solely in terms of the $\hat{T}_i$ operators as

$$\left[(\hat{T}_3-N)+\lambda\left[\frac{N}{Z}\right]^3(\hat{T}_3-\hat{T}_1)^2-\Delta E\left[\frac{N}{Z}\right]^2(\hat{T}_3-\hat{T}_1)\right]\psi=0\ . \tag{2.10}$$

Equation (2.10) represents the algebraically reformulated version of Eq. (2.7). For $\lambda=0$, it reduces to the eigenvalue equation

$$\hat{T}_3\chi_{NLM}(\mathbf{r})=N\chi_{NLM}(\mathbf{r})\ , \tag{2.11}$$

where

$$\chi_{NLM}(\mathbf{r})=2\left[\frac{N-L-1)!}{(N+L)!}\right]^{1/2}e^{-r}(2r)^L\times L_{N-L-1}^{2L+1}(2r)Y_{LM}(\theta,\phi)\ , \tag{2.12}$$

and the N, L, and M satisfy the usual relations of the hydrogen quantum numbers. The $\hat{T}_k$ operators are self-adjoint with respect to the inner product of the Hilbert space $L^2(\mathbb{R}^3,1/r)$. The χ_{nlm} functions form a complete and discrete orthonormal basis satisfying

$$\langle\chi_{nlm}(\mathbf{r})\,|\,\chi_{n'l'm'}(\mathbf{r})\rangle=\int\chi^*_{nlm}(\mathbf{r})\frac{1}{r}\chi_{n'l'm'}(\mathbf{r})d\mathbf{r}=\delta_{nn'}\delta_{ll'}\delta_{mm'}\ . \tag{2.13}$$

The bra-ket notation of Eq. (2.13) is understood to represent this so(4,2) inner product for the remainder of this section. The χ_{nlm} are Coulomb Sturmian functions[25] and are identical to those functions employed by Hylleraas[26] in his classic treatment of ground-state helium by configuration interaction. Their relation to the hydrogenic eigenfunctions of (2.1) is given explicitly by the formula

$$\psi_{nlm}(r,\theta,\phi)=\frac{Z^{3/2}}{n^2}\chi_{nlm}(Zr/n,\theta,\phi)\ . \tag{2.14}$$

The matrix elements of the $\hat{T}_k$ operators in the χ_{nlm} basis [as well as all other elements of so(4,2) in this realization] are obtainable from representation theory.[18] For the treatment of radial problems such as Eq. (2.7), it is sufficient to know that

$$r\chi_{nlm}=(\hat{T}_3-\hat{T}_1)\chi_{nlm}$$
$$=-\tfrac{1}{2}[(n+l)(n-l-1)]^{1/2}\chi_{n-1,l,m}+n\chi_{nlm}$$
$$-\tfrac{1}{2}[(n+l+1)(n-l)]^{1/2}\chi_{n+1,l,m}\ , \tag{2.15}$$

from which all other required matrix elements are obtainable. For more complicated perturbations involving the Cartesian coordinates x, y, or z operators of the larger so(4,2) Lie algebra must be employed.

Here we remark that Eq. (2.10) may be written in the generic form

$$(\hat{K}_N+\lambda\hat{W}-\Delta E\,\hat{S})\psi=0\ . \tag{2.16}$$

In the χ_{nlm} basis, $\hat{K}_N$ is diagonal with eigenvalues $k-N$, $k=1,2,3,\ldots$. For this problem the (infinite) matrix representation of $\hat{W}$ is pentadiagonal and that of $\hat{S}$ tridiagonal, by Eq. (2.15). This close packing is important, as it ensures that all summations in perturbation theory are finite. Equation (2.16) is formally equivalent to an eigenvalue problem defined over a nonorthogonal basis with overlap matrix $\underline{S}$. Both variational and perturbation treatments of such problems have been quite successful in the study of the Zeeman effect for ground-state hydrogen.[19]

As mentioned earlier, the radial nature of the perturbation in (2.8) simplifies perturbation theory. The angular momentum operator $\hat{L}$ and its projection $\hat{L}_z$ commute with $\hat{W}$. Perturbation theory (as well as the variational method) of Eq. (2.3) may be formulated over the subspace of basis functions χ_{nLM} with fixed L and M [cf. Eq. (2.15)]. Moreover, $E_{NLM}(\lambda)$ is $(2L+1)$-fold degenerate with respect to M, and so this index may, in principle, be suppressed in the perturbation expansions. Nondegenerate RSPT is sufficient here and the unperturbed operator $\hat{K}$ of (2.16), defined by its action

$$\hat{K}_N\chi_{nlm,}=(n-N)\chi_{nlm}\ ,\quad n=1,2,3,\ldots \tag{2.17}$$

is Hermitian with respect to the inner product in (2.13). Its reduced resolvent $\hat{Q}_N$ is defined as $\hat{Q}_N=\hat{P}_N\hat{K}_N^{-1}=\hat{K}_N^{-1}\hat{P}_N$, where $\hat{P}_N=\hat{I}-|\chi_{NLM}\rangle\langle\chi_{NLM}|$ and $\hat{I}$ is the identity operator. Resolution of the identity with respect to the complete and discrete orthonormal basis χ_{nlm} gives, in the fixed-(L,M) subspace,

$$\hat{Q}_N=\sum_n{}'\frac{|\psi_{nLM}\rangle\langle\psi_{nLM}|}{n-N}\ , \tag{2.18}$$

where the prime indicates $n\neq N$.

In the tradition of RSPT, the perturbed wave function is expanded as

$$\psi_{NLM}=\chi_{NLM}+\sum_{k=1}^{\infty}\psi_{NLM}^{(k)}\lambda^k\ , \tag{2.19}$$

where it is assumed that

$$\langle \chi_{NLM} \mid \psi_{NLM} \rangle = 1 \tag{2.20}$$

and $\psi_{NLM} \rightarrow \chi_{NLM}$ as $\lambda \rightarrow 0$. Substitution of (1.2) and (2.19) into Eq. (2.16) and collection of terms in λ^n yields the following set of perturbation formulas:

$$E^{(p)}\langle \chi \mid \hat{S} \mid \chi \rangle = \langle \chi \mid \hat{W} \mid \psi^{(p-1)} \rangle - \sum_{m=1}^{p-1} E^{(m)} \langle \chi \mid \hat{S} \mid \psi^{(p-m)} \rangle , \quad p = 1,2,3,\ldots \tag{2.21}$$

$$\psi^{(p)} = -\hat{Q}\hat{W}\psi^{(p-1)} + \sum_{m=1}^{p} E^{(m)} \hat{Q}\hat{S}\psi^{(m)} , \quad p = 1,2,3,\ldots \tag{2.22}$$

where the subscripts N, L, and M have been omitted for notational convenience. In the case $\hat{S} = \hat{I}$, Eqs. (2.21) and (2.22) reduce to the usual RSPT formulas.[27] For this particular problem, the first-order energy is given by

$$E^{(1)}_{NLM} = \frac{N}{Z} \frac{\langle \chi_{NLM} \mid r^2 \mid \chi_{NLM} \rangle}{\langle \chi_{NLM} \mid r \mid \chi_{NLM} \rangle} = \frac{1}{2Z}[3N^2 - L(L+1)] . \tag{2.23}$$

As expected, the result in (2.23) is precisely the expectation value $\bar{r}$ with respect to the hydrogenic basis.[4]

The usual procedure is to now expand the higher-order wave functions $\psi^{(p)}_{NLM}$ in terms of the complete basis χ_{nlm},

$$\psi^{(p)}_{NLM} = \sum_{n}{}' C^{(p)}_{n} \chi_{nLM} , \quad p = 1,2,3,\ldots . \tag{2.24}$$

Since we are working within a fixed-(L,M) subspace, these indices will be suppressed in the Fourier coefficients, which are given by

$$C^{(p)}_{n} = \langle \chi_{nLM} \mid \psi^{(p)}_{NLM} \rangle , \quad C^{(p)}_{N} = 0 , \tag{2.25}$$

and where the inner product of Eq. (2.13) is understood. The latter relation follows from (2.20). Substitution of (2.24) into Eqs. (2.21) and (2.22) yields a recursive procedure formulated entirely in terms of the expansion coefficients $C^{(p)}_{n}$, the $E^{(p)}$, and the matrix elements of $\hat{W}$ and $\hat{S}$. At this point, however, it is convenient to formulate these recursion relations over an unnormalized so(4,2) basis to remove all square roots occurring in matrix elements such as Eq. (2.15). This procedure facilitates the calculation of all $E^{(n)}$ in multiple precision, which will be discussed in Sec. III. As well, it permits all calculations to be performed by symbolic manipulation routines such as MACSYMA which could then compute the $E^{(n)}$ in exact rational form.

We consider the unperturbed basis functions defined by

$$\phi_{NLM} = \left[\frac{(N+L)!}{(N-L-1)!} \right]^{1/2} \chi_{NLM} . \tag{2.26}$$

The resolvent operator $\hat{Q}_N$ in Eq. (2.18) now becomes

$$\hat{Q}_N = \sum_{n}{}' \frac{(n-L-1)!}{(n+L)!} \frac{|\phi_{nLM}\rangle\langle\phi_{nLM}|}{n-N} . \tag{2.27}$$

The matrix elements of $\hat{S} = (N/Z)^2 r$ and $\hat{W} = (N/Z)^3 r^2$ in this basis are easily determined. We now write

$$\psi^{(p)}_{NLM} = \sum_{n\,(\neq N)} D^{(p)}_{n} \phi_{nLM} , \tag{2.28}$$

and modify (2.20) accordingly. Substitution of (2.28) into Eqs. (2.21) and (2.22) yields the following recursion formulas:

$$E^{(p)}_{NLM} = \frac{1}{4Z}\{(N-L-1)(N-L-2)D^{(p-1)}_{N-2} - 2(N-L-1)(2N-1)D^{(p-1)}_{N-1} + 2[3N^2 - L(L+1)]D^{(p-1)}_{N} - 2(N+L+1)(2N+1)D^{(p-1)}_{N+1} + (N+L+1)(N+L+2)D^{(p-1)}_{N+2}\} + \frac{1}{2N}\sum_{m=1}^{p-1} E^{(m)}_{NLM}[(N-L-1)D^{(p-m)}_{N-1} + (N+L+1)D^{(p-m)}_{N+1}] , \tag{2.29}$$

$$D^{(p)}_{n} = \frac{1}{4(N-n)} \left\{ \left[\frac{N}{Z} \right]^3 [(n-L-1)(n-L-2)D^{(p-1)}_{N-2} - 2(n-L-1)(2n-1)D^{(p-1)}_{N-1} + 2[3n^2 - L(L+1)]D^{(p-1)}_{N} - 2(n+L+1)(2n+1)D^{(p-1)}_{N+1} + (n+L+1)(n+L+2)D^{(p-1)}_{N+2}] + 2\left[\frac{N}{Z} \right]^2 \sum_{m=1}^{p} E^{(m)}_{NLM}[(n-L-1)D^{(p-1)}_{N-1} - 2nD^{(p-m)}_{N} + (n+L+1)D^{(p-m)}_{N+1}] \right\} , \quad n \neq N . \tag{2.30}$$

The initial value of this recursion procedure is, simply, $D_N^{(0)}=1$, representing the unperturbed wave function, χ_{NLM}. From this, one calculates $E^{(1)}$, then $\psi^{(1)}$, $E^{(2)}$, $\psi^{(2)}$, etc., in the usual manner. The finite summations involved in each order of perturbation theory are a consequence of the close-packed representations of $\hat{W}$ and $\hat{S}$ in the χ_{nlm} basis. In fact, the $D_n^{(p)}$ may be nonzero only if $n \geq L+1$ and $n \leq N+2p$. The expansion coefficients may be stored in a row vector to economize on the computer-memory requirements. The RS procedure described above is easily computer coded to determine perturbation expansions for general states. In this way, the coefficients $E_{NL0}^{(n)}$ have been calculated for the levels $1 \leq N \leq 4$, $0 \leq L \leq N-1$ to order $n \sim 100$. The first 91 coefficients of the ground-state series are presented in Table I.

In standard RSPT, a knowledge of perturbation energies $E^{(i)}$ and wave functions $\psi^{(i)}$ to order n actually determines the $E^{(i)}$ to order $2n+1$.[28] Explicit calculation of these coefficients may be accomplished by a sequence of transformations of the RSPT perturbation equations. Such a procedure has been formulated for the case of intermediate normalization in Eq. (2.20).[29] Its generalization to the nonorthogonal perturbation problem (2.16) is given by

TABLE I. The first 90 (scaled) coefficients $E_{NLM}^{(n)}$ of the Rayleigh-Schrödinger perturbation expansion of $E(\lambda)$ for the ground state of the hydrogen atom in a linear radial potential, $(N,L,M)=(1,0,0)$.

n	$100^{-n}E^{(n)}$	n	$100^{-n}E^{(n)}$
0	$-0.500\,000\,000\,000\,000\,000\,000\,000\,000\,000\,00$	46	$-0.821\,688\,501\,395\,158\,459\,391\,949\,301\,036\,44\times10^{-25}$
1	$0.150\,000\,000\,000\,000\,000\,000\,000\,000\,000\,00\times10^{-1}$	47	$0.593\,229\,850\,182\,382\,248\,435\,615\,743\,725\,98\times10^{-25}$
2	$-0.150\,000\,000\,000\,000\,000\,000\,000\,000\,000\,00\times10^{-3}$	48	$-0.437\,161\,715\,820\,093\,184\,118\,077\,987\,500\,67\times10^{-25}$
3	$0.675\,000\,000\,000\,000\,000\,000\,000\,000\,000\,00\times10^{-5}$	49	$0.328\,690\,365\,668\,158\,544\,356\,256\,668\,662\,61\times10^{-25}$
4	$-0.496\,875\,000\,000\,000\,000\,000\,000\,000\,000\,00\times10^{-6}$	50	$-0.252\,050\,073\,320\,727\,488\,936\,720\,711\,745\,99\times10^{-25}$
5	$0.480\,375\,000\,000\,000\,000\,000\,000\,000\,000\,00\times10^{-7}$	51	$0.197\,050\,461\,238\,217\,396\,037\,478\,745\,061\,40\times10^{-25}$
6	$-0.558\,299\,999\,999\,999\,999\,999\,999\,999\,999\,99\times10^{-8}$	52	$-0.157\,000\,403\,752\,759\,739\,367\,340\,422\,495\,40\times10^{-25}$
7	$0.745\,573\,359\,374\,999\,999\,999\,999\,999\,999\,99\times10^{-9}$	53	$0.127\,439\,624\,870\,074\,186\,178\,559\,489\,608\,85\times10^{-25}$
8	$-0.111\,431\,933\,496\,093\,750\,000\,000\,000\,000\,00\times10^{-9}$	54	$-0.105\,351\,763\,554\,695\,969\,031\,135\,001\,591\,17\times10^{-25}$
9	$0.183\,291\,714\,404\,296\,875\,000\,000\,000\,000\,00\times10^{-10}$	55	$0.886\,688\,668\,236\,233\,859\,895\,309\,834\,303\,20\times10^{-26}$
10	$-0.328\,051\,587\,371\,337\,890\,624\,999\,999\,999\,99\times10^{-11}$	56	$-0.759\,549\,138\,820\,891\,270\,980\,423\,857\,040\,33\times10^{-26}$
11	$0.633\,670\,455\,014\,318\,847\,656\,249\,999\,999\,98\times10^{-12}$	57	$0.662\,009\,148\,068\,409\,199\,743\,461\,405\,188\,34\times10^{-26}$
12	$-0.131\,294\,601\,381\,998\,199\,462\,890\,625\,000\,00\times10^{-12}$	58	$-0.586\,905\,230\,570\,875\,497\,511\,415\,393\,742\,93\times10^{-26}$
13	$0.290\,407\,932\,815\,958\,874\,511\,718\,749\,999\,99\times10^{-13}$	59	$0.529\,108\,267\,227\,319\,246\,969\,318\,727\,053\,03\times10^{-26}$
14	$-0.683\,045\,342\,904\,476\,692\,199\,707\,031\,249\,97\times10^{-14}$	60	$-0.484\,924\,826\,996\,715\,787\,012\,196\,759\,027\,41\times10^{-26}$
15	$0.170\,268\,828\,630\,796\,075\,922\,012\,329\,101\,56\times10^{-14}$	61	$0.451\,691\,744\,556\,058\,543\,774\,309\,354\,475\,15\times10^{-26}$
16	$-0.448\,555\,463\,827\,030\,484\,123\,218\,059\,539\,78\times10^{-15}$	62	$-0.427\,499\,837\,911\,959\,990\,278\,175\,143\,521\,36\times10^{-26}$
17	$0.124\,560\,012\,753\,220\,375\,180\,089\,354\,515\,07\times10^{-15}$	63	$0.411\,005\,382\,623\,195\,535\,002\,087\,173\,355\,13\times10^{-26}$
18	$-0.363\,757\,070\,084\,564\,442\,546\,386\,441\,588\,38\times10^{-16}$	64	$-0.401\,302\,463\,530\,579\,679\,888\,543\,864\,394\,93\times10^{-26}$
19	$0.111\,476\,957\,302\,336\,220\,743\,983\,378\,186\,82\times10^{-16}$	65	$0.397\,838\,750\,078\,773\,939\,300\,464\,786\,959\,38\times10^{-26}$
20	$-0.357\,798\,342\,931\,711\,740\,037\,247\,069\,731\,71\times10^{-17}$	66	$-0.400\,363\,508\,519\,466\,279\,332\,814\,088\,894\,21\times10^{-26}$
21	$0.120\,051\,857\,638\,413\,444\,638\,039\,124\,687\,75\times10^{-17}$	67	$0.408\,900\,975\,575\,062\,142\,297\,520\,742\,461\,24\times10^{-26}$
22	$-0.420\,365\,800\,567\,908\,633\,696\,136\,702\,983\,86\times10^{-18}$	68	$-0.423\,745\,346\,676\,736\,849\,702\,780\,785\,568\,50\times10^{-26}$
23	$0.153\,360\,143\,295\,769\,147\,231\,101\,361\,067\,15\times10^{-18}$	69	$0.445\,476\,097\,796\,335\,311\,037\,748\,438\,766\,24\times10^{-26}$
24	$-0.582\,059\,406\,890\,645\,188\,347\,842\,489\,824\,93\times10^{-19}$	70	$-0.474\,994\,540\,774\,779\,878\,841\,430\,677\,435\,61\times10^{-26}$
25	$0.229\,496\,413\,047\,783\,031\,266\,743\,250\,407\,61\times10^{-19}$	71	$0.513\,584\,717\,056\,957\,188\,535\,242\,986\,099\,96\times10^{-26}$
26	$-0.938\,772\,773\,265\,986\,216\,651\,723\,463\,535\,45\times10^{-20}$	72	$-0.563\,004\,260\,158\,345\,860\,211\,196\,378\,440\,93\times10^{-26}$
27	$0.397\,904\,294\,077\,082\,596\,593\,212\,562\,900\,57\times10^{-20}$	73	$0.625\,614\,035\,926\,645\,501\,887\,887\,835\,794\,53\times10^{-26}$
28	$-0.174\,550\,321\,548\,882\,772\,531\,493\,982\,016\,43\times10^{-20}$	74	$-0.704\,559\,624\,709\,560\,921\,017\,302\,771\,311\,04\times10^{-26}$
29	$0.791\,602\,639\,259\,323\,210\,982\,147\,667\,136\,90\times10^{-21}$	75	$0.804\,023\,621\,541\,125\,555\,849\,224\,055\,356\,31\times10^{-26}$
30	$-0.370\,755\,066\,788\,492\,883\,167\,441\,755\,864\,90\times10^{-21}$	76	$-0.929\,576\,132\,056\,377\,148\,379\,046\,721\,318\,33\times10^{-26}$
31	$0.179\,157\,464\,815\,671\,334\,924\,065\,702\,168\,97\times10^{-21}$	77	$0.108\,866\,295\,652\,818\,586\,451\,597\,416\,096\,86\times10^{-25}$
32	$-0.892\,378\,966\,577\,822\,308\,315\,422\,374\,289\,95\times10^{-22}$	78	$-0.129\,128\,860\,654\,589\,809\,294\,144\,242\,810\,29\times10^{-25}$
33	$0.457\,774\,048\,732\,210\,306\,549\,534\,491\,236\,83\times10^{-22}$	79	$0.155\,097\,723\,619\,677\,465\,429\,090\,346\,997\,23\times10^{-25}$
34	$-0.241\,647\,201\,453\,735\,762\,946\,086\,139\,338\,28\times10^{-22}$	80	$-0.188\,613\,296\,368\,924\,774\,994\,135\,519\,862\,99\times10^{-25}$
35	$0.131\,160\,011\,205\,232\,745\,599\,460\,912\,132\,35\times10^{-22}$	81	$0.232\,197\,828\,747\,785\,697\,640\,161\,847\,694\,07\times10^{-25}$
36	$-0.731\,455\,825\,158\,693\,970\,560\,026\,253\,607\,89\times10^{-23}$	82	$-0.289\,333\,517\,676\,075\,736\,986\,089\,338\,689\,89\times10^{-25}$
37	$0.418\,828\,252\,977\,178\,533\,701\,552\,958\,848\,37\times10^{-23}$	83	$0.364\,864\,313\,826\,220\,252\,439\,876\,968\,030\,34\times10^{-25}$
38	$-0.246\,067\,597\,977\,802\,569\,592\,747\,045\,140\,54\times10^{-23}$	84	$-0.465\,580\,581\,744\,929\,365\,930\,677\,981\,479\,26\times10^{-25}$
39	$0.148\,240\,529\,384\,157\,055\,419\,799\,490\,396\,07\times10^{-23}$	85	$0.601\,075\,963\,679\,301\,727\,165\,278\,337\,564\,82\times10^{-25}$
40	$-0.915\,187\,648\,114\,411\,505\,275\,783\,023\,345\,87\times10^{-24}$	86	$-0.785\,012\,325\,307\,182\,893\,184\,000\,388\,602\,32\times10^{-25}$
41	$0.578\,672\,493\,942\,687\,663\,895\,642\,511\,414\,87\times10^{-24}$	87	$0.103\,700\,083\,948\,416\,323\,576\,906\,644\,008\,62\times10^{-24}$
42	$-0.374\,537\,474\,461\,043\,538\,311\,658\,984\,867\,41\times10^{-24}$	88	$-0.138\,541\,998\,709\,455\,738\,348\,593\,170\,465\,79\times10^{-24}$
43	$0.248\,009\,542\,735\,975\,891\,923\,421\,355\,351\,86\times10^{-24}$	89	$0.187\,166\,849\,000\,653\,892\,863\,822\,970\,985\,14\times10^{-24}$
44	$-0.167\,931\,860\,627\,019\,886\,826\,310\,665\,247\,16\times10^{-24}$	90	$-0.255\,663\,175\,708\,616\,540\,819\,861\,497\,262\,43\times10^{-24}$
45	$0.116\,219\,682\,254\,759\,482\,148\,138\,704\,353\,57\times10^{-24}$		

$$E^{(a+b+1)}\langle\chi\,|\,\hat{S}\,|\,\chi\rangle=\langle\psi^{(a)}\,|\,\hat{W}\,|\,\psi^{(b)}\rangle-\sum_{i=1}^{a}\sum_{j=1}^{b}E^{(a+b+1-i-j)}\langle\psi^{(i)}\,|\,\hat{S}\,|\,\psi^{(j)}\rangle$$
$$-\sum_{i=1}^{a}\langle\chi\,|\,\hat{S}\,|\,\psi^{(i)}\rangle E^{(a+b+1-i)}-\sum_{j=1}^{b}\langle\chi\,|\,\hat{S}\,|\,\psi^{(j)}\rangle E^{(a+b+1-j)}\,, \tag{2.31}$$

where a and b are arbitrary non-negative integers. For $a=b=n$, we have the desired result. If the expansions in (2.19) and (2.20) are now invoked, Eq. (2.31) may be formulated in terms of the expansion coefficients $C_n^{(p)}$ or $D_n^{(p)}$, the $E^{(p)}$, and the matrix elements of $\hat{W}$ and $\hat{S}$.

III. LARGE-ORDER PERTURBATION THEORY (LOPT)

As mentioned earlier, Mehta and Patil[7] performed the first Bender-Wu analysis of (1.1) to ascertain the large-order behavior of the perturbation coefficients $E_{NLM}^{(n)}$, but only for the case $L=0$. In this case, the WKB integral encountered in the tunneling factor is related to that of the quartic-anharmonic-oscillator problem. For nonzero L states, this integral becomes complicated due to the presence of the centrifugal-barrier term. Harrell and Simon[6] determined the asymptotics of the tunneling factor, hence $\mathrm{Im}E$, by a clever selection of turning points and partitioning of the interval under the barrier. They did not, however, proceed to develop the actual asymptotics of the perturbation coefficients $E^{(n)}$.

In this section we employ the usual WKB methods and dispersion techniques of Bender-Wu theory[30] to develop the LOPT formulas for the expansions in (1.2) for $Z=1$. The asymptotics of the tunneling factor will be determined using elliptic integrals, a method different from that employed in Ref. 6. The present procedure was motivated by a study[31] of the WKB (semiclassical) eigenvalue expressions for (1.1) which employed elliptic functions. An interesting result of this section is that some complicated angular-quantum-number-dependent terms occurring in the tunneling factor integral vanish in the final LOPT formulas, in accord with numerical analysis. We finally mention that a Bender-Wu WKB analysis of (1.1) is relatively simple due to its spherical symmetry. For more complicated atomic problems such as the quadratic Zeeman effect in hydrogen, a difficult multidimensional analysis must be devised.[32]

For the dispersion methods of Bender-Wu theory to be rigorously applicable,[33] $E(\lambda)$ must satisfy the properties of a Stieltjes function. This was shown by Simon[34] in his detailed analysis of the quartic anharmonic oscillator. The four properties are the following:

(i) $E(\lambda)$ is analytic in the cut plane $|\arg\lambda|<\pi$;
(ii) $E(\lambda)$ is real for λ real and positive;
(iii) $E(\lambda)$ has the Herglotz property, i.e., $\mathrm{Im}E>0$ when $\mathrm{Im}\lambda>0$ and $\mathrm{Im}E<0$ when $\mathrm{Im}\lambda<0$; and
(iv) the perturbation series (1.2) is an asymptotic expansion valid uniformly.

Property (ii) follows from the Hermiticity of $\hat{H}^{(0)}=-\frac{1}{2}\nabla^2-r^{-1}$ and $\hat{V}=r$. Property (iii) may be derived in virtually the same way as for the quartic anharmonic oscillator,[35] i.e., by multiplying (1.1) by $\psi^*(\mathbf{r})$, integrating over r by parts, and showing that $\mathrm{Im}E/\mathrm{Im}\lambda>0$. We do not intend to prove (i) and (iv) here. Concerning (i), it has been shown[7] that $\lambda=0$ is a singular point of $E(\lambda)$, accounting for the divergence of the perturbation series. As will be shown below, $E(\lambda)$ is complex for λ real and negative. From (iii) it follows that $E(\lambda)$ has a branch cut along the negative real axis. Presumably, a differential equation analysis analogous to that of Ref. 35 could be used to prove (i). As for (iv), the perturbation of discrete hydrogenic states could be handled by the techniques outlined in Appendix II of Simon.[34]

A final and important property of the charmonium problem is

$$\text{(v)}\quad E(\lambda)\sim F\lambda^{2/3}\ \text{as}\ \lambda\to\infty\,. \tag{3.1}$$

This may be shown by a Symanzik-type transformation[34] of (1.1) (cf. Appendix B) which effectively reverses the roles of the Coulomb and linear potentials. Properties (i)—(v) qualify that the perturbation series in (2.1) is negative Stieltjes for $n\geq 1$, i.e., that[34]

$$E_{NLM}^{(n)}=\frac{1}{\pi}\int_{-\infty}^{0}\frac{\mathrm{Im}E_{NLM}(\lambda+i0)}{\lambda^{n+1}}d\lambda\,,\quad n\geq 1\,. \tag{3.2}$$

For n very large, the major contribution to this integral comes from the region $\lambda\sim 0$. Bender-Wu theory employs WKB techniques to approximate $\mathrm{Im}[E(\lambda)]$ for $\lambda\to 0^-$. Its application to the hydrogenic problem (1.1) for $Z=1$ is developed below (the extension to arbitrary Z is obtained by scaling).

We first substitute $\mathbf{r}=\frac{1}{2}\mathbf{r}'$ in (1.1) and drop the primes to produce the modified eigenvalue problem

$$\left[-\nabla^2-\frac{1}{r}+\beta r\right]\psi(\tfrac{1}{2}\mathbf{r})=\bar{E}\psi(\tfrac{1}{2}\mathbf{r})\,, \tag{3.3}$$

where $\beta=\lambda/4$, $\bar{E}=\frac{1}{2}E$, and the unperturbed eigenvalues are given by $\bar{E}_{NLM}^{(0)}=-(4N^2)^{-1}$. The substitution $\psi=r^{-1}\xi(r)Y_{LM}(\theta,\phi)$ yields the radial equation

$$\left[-\frac{d^2}{dr^2}+\frac{G^2}{r^2}-\frac{1}{r}+\beta r-\bar{E}\right]\xi(r)=0\,, \tag{3.4}$$

where $G^2=L(L+1)$. In order to study the asymptotics of $\mathrm{Im}E$ for $\lambda\to 0^-$, we assume that $\beta=-\epsilon$, with $0<\epsilon\ll 1$. The unstable potential is sketched in Fig. 1 for nonzero L. The classical turning points are given by the roots of the cubic equation

$$r^3-\frac{W}{\epsilon}r^2+\frac{1}{\epsilon}r-\frac{G^2}{\epsilon}=0\,, \tag{3.5}$$

where $W\equiv-\bar{E}$. The roots are approximated by the asymptotic formulas

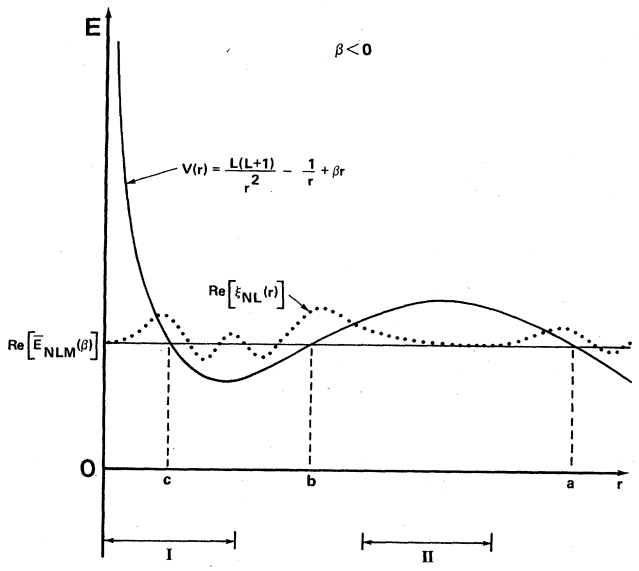

FIG. 1. An unstable charmonium potential corresponding to a negative coupling constant β in Eq. (3.4), for an arbitrary nonzero value of the angular momentum L. The radial wave function $\xi_{NL}(r)$ is superimposed on the energy scale and represents a tunneling state. The classical turning points a, b, and c are also shown. In region I, the wave function is well represented by its unperturbed hydrogenic counterpart. In region II, a first-order WKB approximation is employed.

$$a \sim W\epsilon^{-1} - W^{-1} ,$$
$$b \sim (1+\gamma)(2W)^{-1} , \tag{3.6}$$
$$c \sim (1-\gamma)(2W)^{-1} ,$$

where

$$\gamma = (1-4G^2W)^{1/2} \tag{3.7}$$

and the approximations for b and c are obtained by setting $\epsilon=0$. Note that $a+b+c=W/\epsilon$, as required. Also, $c\to 0$ as $G\to 0$.

Near $r=0$ (region I in Fig. 1), the radial wave function $\xi(r,\lambda)$ is well approximated by $rR_{NL}(r)$, where $R_{NL}(r)$ is the (unperturbed) hydrogen radial function. Under the potential barrier (region II in Fig. 1), $b<r<a$, the wave function is approximated by the first-order WKB function,

$$\xi^{\mathrm{II}}(r) = C_1 \left[W + \frac{G^2}{r^2} - \frac{1}{r} - \epsilon r \right]^{-1/4} \times \exp\left[-\int_b^r \left[W + \frac{G^2}{x^2} - \frac{1}{x} - \epsilon x \right]^{1/2} dx \right] . \tag{3.8}$$

The constant C_1 is obtained by the matching condition $\xi^{\mathrm{I}}(r) \sim \xi^{\mathrm{II}}(r)$, $r \gg b$. Since[36]

$$\xi^{(\mathrm{I})}(r) \sim \frac{1}{N^{N+1}[2(N+L)!(N-L-1)!]^{1/2}} e^{-r/2N} r^N \quad \text{as } r\to\infty , \tag{3.9}$$

the matching condition yields

$$C_1 = \frac{N^{N-3/2}\gamma^N}{2[(N+L)!(N-L-1)!]^{1/2}} \times \left[\frac{(2GW^{1/2}-1)(1+\gamma)}{4G^2W-1-\gamma} \right]^{-G} , \tag{3.10}$$

where the integral in (3.8) has been evaluated to zeroth order in ϵ.[37]

We now proceed to obtain the leading asymptotics of $\mathrm{Im}E$ using the WKB function (3.8).[30] First, multiply Eq. (3.4) by $\xi^*(r)$ and subtract its complex conjugate. Then integrate the result from $r=0$ to a point beyond the outermost turning point at $r=a$ (to avoid reflections of current back toward $r=0$) to obtain

$$\mathrm{Im}\bar{E} = \frac{(2i)^{-1}\left[-\xi^*(r)\frac{d}{dr}\xi(r) + \xi(r)\frac{d}{dr}\xi^*(r) \right]}{\int_0^r \xi^*(x)\xi(x)dx} = \frac{J(r)}{N(r)} . \tag{3.11}$$

The numerator $J(r)$ is the *current density*[38] of $\xi(r)$ at a point r. By conservation of probability, the right-hand side (rhs) of (3.11) is independent of r. The WKB wave function (3.8) is now substituted into Eq. (3.11). In order to avoid the difficulties associated with the outer turning point, the path of integration along the real axis is deformed to travel around the point clockwise. This semicircular path is then shrunk to zero. The WKB integral splits into two parts and, after some algebraic manipulations, the current density becomes

$$J(r) = C_1^2 \exp(-2I_{ba}) , \tag{3.12}$$

where I_{ba}, the tunneling factor, is given by

$$I_{ba} = \int_b^a \left[W + \frac{G^2}{x^2} - \frac{1}{x} - \epsilon x \right]^{1/2} dx . \tag{3.13}$$

In order to evaluate (3.13) to leading order in ϵ as $\epsilon\to 0$, we write it as

$$I_{ba} = \epsilon^{1/2} \int_b^a x^{-1} \left[-x^3 + \frac{W}{\epsilon}x^2 - \frac{1}{\epsilon}x + \frac{G^2}{\epsilon} \right]^{1/2} dx$$
$$= \epsilon^{1/2} \int_b^a x^{-1}[(a-x)(x-b)(x-c)]^{1/2} dx$$
$$= -\epsilon^{1/2} \int_b^a \frac{(x^2 - Wx/\epsilon - 1/\epsilon - G^2/\epsilon x)}{[(a-x)(x-b)(x-c)]^{1/2}} dx . \tag{3.14}$$

After some further manipulations, the final integral in (3.14) may be written as

$$I_{ba} = g\epsilon^{-1/2} \left[\left(-\frac{2}{3} + \frac{G^2}{c} + \frac{1}{3}Wc \right) K(k) + \tfrac{1}{3}W(a-c)E(k) - G^2(c^{-1}-b^{-1})\Pi(\alpha^2,k) \right] , \tag{3.15}$$

where $K(k)$, $E(k)$, and $\Pi(\alpha^2,k)$ are the complete elliptic integrals of, respectively, the first, second, and third kind,[39] and

$$k^2=\frac{a-b}{a-c}\ ,\quad (k')^2=1-k^2=\frac{b-c}{a-c}\ ,$$
$$\alpha^2=\frac{ck^2}{b}\ ,\quad g=\frac{2}{(a-c)^{1/2}}\ . \tag{3.16}$$

From (3.6) it follows that

$$(k')^2\sim\gamma W^{-2}\epsilon\ ,\quad \epsilon\to 0\ . \tag{3.17}$$

The asymptotics of the elliptic integrals are given by[40]

$$K(k)\sim\ln\left[\frac{4}{k'}\right]\quad\text{as }\epsilon\to 0\ , \tag{3.18a}$$

$$E(k)\sim 1+\left[\tfrac{1}{2}\ln\left[\frac{4}{k'}\right]-\tfrac{1}{2}\right](k')^2\quad\text{as }\epsilon\to 0\ , \tag{3.18b}$$

and

$$\Pi(\alpha^2,k)\sim\frac{1}{1-\alpha^2}\left[\ln\left[\frac{4}{k'}\right]+(-\alpha^2)^{1/2}\arctan^{-1}[(-\alpha^2)^{1/2}]\right]$$
$$=\frac{1}{1-\alpha^2}\ln\left[\frac{4}{k'}\right]+\frac{\alpha}{2(1-\alpha^2)}\ln\left|\frac{1-\alpha}{1+\alpha}\right|\quad\text{as }\epsilon\to 0\ . \tag{3.18c}$$

The argument of the second logarithm in (3.18c) may be written as

$$\frac{1-\alpha}{1+\alpha}=\frac{(2GW^{1/2}-1)(1-\gamma)}{4G^2W-1+\gamma}=\frac{(2GW^{1/2}-1)(1+\gamma)}{4G^2W-1-\gamma}\ . \tag{3.19}$$

After some more algebraic manipulations, we find that

$$I_{ba}\sim\frac{2W^{1/2}}{3\epsilon}-\frac{1}{W^{1/2}}\ln\left[\frac{4W}{\epsilon^{1/2}}\right]+\frac{1}{2W^{1/2}}\ln\gamma^2-G\ln\left[\frac{(2GW^{1/2}-1)(1+\gamma)}{4G^2-1-\gamma}\right]\quad\text{as }\epsilon\to 0\ . \tag{3.20}$$

This equation is essentially the result obtained by Harrell and Simon,[6] apart from a factor which has automatically been absorbed by our normalization constant C_1. Equation (3.20) is now substituted into Eq. (3.12) to give

$$J(r)\sim\frac{N^{2N-3}}{4(N+L)!(N-L-1)!}\left[\frac{4W}{\epsilon^{1/2}}\right]^{2W-1/2}\times\exp\left[-\frac{4W^{3/2}}{3\epsilon}\right]\quad\text{as }\epsilon\to 0\ . \tag{3.21}$$

If we now choose r large enough in Eq. (3.11), i.e., $r\gg a$, then to zeroth order in ϵ, $N(r)=1$ so that $\mathrm{Im}\bar{E}=J(r)$. It is now tempting to simply substitute $W=\bar{E}^{(0)}$ into (3.21). As in the Stark effect,[41] however, the exponential in (3.21) contributes two significant terms to the asymptotics of $J(r)$, since

$$W^{3/2}=[-\bar{E}^{(0)}-\bar{E}^{(1)}\epsilon+O(\epsilon^2)]^{3/2}=(-\bar{E}^{(0)})^{3/2}+\tfrac{3}{2}(-\bar{E}^{(0)})^{1/2}\bar{E}^{(1)}\epsilon+O(\epsilon^2)\quad\text{as }\epsilon\to 0\ . \tag{3.22}$$

From $\bar{E}^{(1)}_{NLM}=3N^2-L(L+1)$, we have the final result

$$\mathrm{Im}[\bar{E}_{NLM}(\epsilon)]\sim\frac{N^{-6N-3}}{4(N+L)!(N-L-1)!}\epsilon^{-2N}\times\exp\left[-\frac{1}{6N^3\epsilon}-3N+\frac{L(L+1)}{N}\right]\quad\text{as }\epsilon\to 0\ , \tag{3.23}$$

for the scaled problem (3.4).

Returning to the unscaled hydrogen perturbation problem (1.1), one finds that for $\lambda<0$, the complex part of the resonance energy is given by

$$\mathrm{Im}[E_{NLM}(\lambda)]\sim\frac{N^{-6N}4^{2N}}{2N^3(N+L)!(N-L-1)!}(-\lambda)^{-2N}\times\exp\left[\frac{2}{3N^2\lambda}-3N+\frac{L(L+1)}{N}\right]\cdot \tag{3.24}$$

Substitution of this result into the dispersion relation (3.2) gives [with change of variable $t=(-\lambda)^{-1}$] the final expression for the large-order behavior of the Rayleigh-Schrödinger perturbation coefficients:

$$E^{(n)}_{NLM}\sim\frac{(-1)^{n+1}3^{2N}2^{2N-1}}{\pi N^3(N+L)!(N-L-1)!}\times\exp\left[-3N+\frac{L(L+1)}{N}\right]\times(\tfrac{3}{2}N^3)^n\Gamma(n+2N)\quad\text{as }n\to\infty\ . \tag{3.25}$$

For $L=0$, Eq. (3.25) agrees with the result of Mehta and Patil.[7] It has also been checked by numerical asymptotic analysis of RS perturbation coefficients for the cases $1\le N\le 3$, $0\le L\le N-1$, $M=0$.

We observe that much of the complicated L-dependent behavior encountered in the normalization constant, Eq. (3.10), and in the tunneling factor integral, Eq. (3.20), has been canceled out in Eq. (3.21), and hence in the final LOPT formula (3.25). It is interesting to note that Eq. (3.25) could have also been obtained by merely performing a Bender-Wu WKB analysis of the simpler $L=0$ case and then simply employing the general first-order perturbation energy correction $\bar{E}^{(1)}=3N^2-L(L+1)$ as in Eq. (3.22).

A remark may now be made concerning the summability of the Stieltjes charmonium perturbation series. The $n!$-type asymptotic behavior of the RS coefficients demonstrated in (3.25) is sufficient to ensure the determinacy of the moment problem associated with Eq. (3.2), by Carleman's theorem (cf. Appendix C). The diagonal

TABLE II. Numerical estimates of the asymptotic constants A_1^{NLM} in the correction factor (3.26) to the Bender-Wu LOPT formulas (3.25). These estimates were obtained by Thiele-Padé extrapolation of high-order perturbation coefficients $E_{NLM}^{(n)}$.

	L			
N	0	1	2	3
1	−5.4444			
2	−14.4444	−14.111 11		
3	−28.1111	−27.962 96	−26.7777	
4	−46.4444	−45.695	−45.6944	−43.4444
5	−69.4444	−69.3911		

sequences of Padé approximants $[N+k,N]$, $k \geq -1$, converge uniformly to $E(\lambda)$ in the limit $N \to \infty$ over compact subsets of the cut plane $|\arg\lambda| < \pi$. This accounts for the Padé convergence of the ground-state series observed in Refs. 8 and 9.

Regarding the LOPT formula (3.25) of charmonium, if higher-order corrections to $\mathrm{Im}[E_{NLM}(\lambda)]$ in Eq. (3.24) are known, the corresponding corrections to the asymptotic behavior of the $E_{NLM}^{(n)}$ could be determined by the dispersion relation (3.2). Such corrections are typically of the form

$$1+\frac{A_1}{n}+\frac{A_2}{n^2}+\cdots \tag{3.26}$$

and relatively consistent numerical results for a number of coefficients can be obtained. An analytic formula for A_1 was determined by Bender and Wu[30] for all levels of the quartic anharmonic oscillator. When corrections of this form are assumed to accompany the LOPT formulas in (3.25), a numerical asymptotic extraction of the A_1 coefficients yields the values given in Table II. The Thiele-Padé method, to be described in Sec. IV, was employed in these calculations (in the variable $z=n^{-1}$, which is similar to Richardson extrapolation). In almost every case, the numerical values strongly suggest that the coefficients are rational. The coefficients corresponding to the cases $(N,L)=(N,0)$ and $(N,L)=(N,N-1)$ behave as

$$A_1^{N00}=-\frac{21N^2+18N+10}{9} \tag{3.27}$$

and

$$A_1^{N,N-1,0}=-\frac{18N^2+24N+7}{9}\ , \tag{3.28}$$

respectively. A general expression which would account for all values in Table II has not yet been conjectured.

IV. CONTINUED FRACTIONS AT LARGE ORDER (CFLO)

After a few expository remarks, we focus on the CF representations of the divergent charmonium perturbation series. Some important properties of continued fractions are outlined in Appendix C.

The RITZ continued fractions provide an ideal representation of many quantum-mechanical perturbation series, especially in the context of LOPT. The coefficients c_n of a CF exist in a one-to-one correspondence with their series counterparts $E^{(n)}$. This is unlike the situation encountered with Padé approximant representations, where each $[N,M]$ Padé approximant possesses its own set of $N+M+1$ coefficients. Moreover, the single sequence $\{c_n\}$ generates the sequence of convergents $\{w_n(z)\}$ of $C(z)$ which constitute the two principal diagonal sequences of Padé approximants to the series. In the case of Stieltjes functions, for which all $c_n>0$ so that $C(z)$ is an S fraction, the stepwise descent of the Padé-approximant table may furnish increasingly more accurate upper and lower bounds on the function concerned.

In addition to these computational aspects, however, much more information appears to be encoded in the coefficients of S-fraction representations. By CFLO, we refer to the behavior of c_n as $n \to \infty$. Preliminary investigations[11] revealed a fundamental relation between CFLO and LOPT in nonrelativistic quantum-mechanical perturbation problems: if $E^{(n)} \sim (-1)^{n+1}(pn)!$ as $n \to \infty$, $p=0,1,2,\ldots$, then $c_n \sim n^p$ as $n \to \infty$. This conjecture has since been proved[42] for $p=0$, 1, and 2 by asymptotic analysis of the quotient-difference (QD) algorithm, introduced in Appendix C. The case $p=1$ is relevant to this study and we state it precisely: If the series in (1.2) is Stieltjes for $n \geq 1$ and

$$E^{(n)} \sim (-1)^{n+1} A\,\Gamma(n+\alpha)k^n\left[1+O\left[\frac{1}{n}\right]\right] \quad \text{as } n \to \infty\ , \tag{4.1a}$$

where A, α, and k are constants independent of n, then for its S-fraction representation (1.3),

$$c_n \sim \tfrac{1}{2}kn \quad \text{as } n \to \infty\ . \tag{4.1b}$$

An S fraction whose coefficients grow as $c_n \sim n^p$, as $n \to \infty$, will be referred to as an $S_{(p)}$ fraction. From Eq. (C10) in Appendix C, $S_{(p)}$ fractions automatically converge in the cut plane $|\arg z| < \pi$ for $p \leq 2$.

The coefficients c_n^{NL0} have been calculated from the RS coefficients $E_{NL0}^{(n)}$ to $n=100$ for the ground state and to $n=90$ for the excited states $N=2,3$ and $0 \leq L \leq N-1$. Practical calculations of RITZ continued-fraction coefficients from formal power series are impeded by the numerical instability of algorithms such as the QD scheme. 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), the coefficients are meaningless after about c_{60}. As a result, all calculations of the $E^{(n)}$ and c_n have been performed in multiple precision.[43] Each decimal number is represented by typically 200 digits in these calculations (as a vector in single precision), which would ensure a 32-digit accuracy of the c_n to at least $n=100$. The coefficients c_n^{100} of the ground-state representation are presented in Table III, accurate to all digits shown. An immediate observation of these coefficients is that they are all positive, a consequence of the Stieltjes nature of the perturbation series discussed in Sec. III.

From Eqs. (4.1) and (3.25), it is expected that $c_n^{NL0} \to \frac{3}{4}N^3 n$ as $n \to \infty$, which is observed numerically.

TABLE III. The first 100 coefficients c_n of the S-fraction repreentation, Eq. (1.3), of the ground-state Rayleigh-Schrödinger perturbation series for $E(\lambda)$.

n	c_n	n	c_n
1	$0.150\,000\,000\,000\,000\,000\,000\,000\,000\,000\,00\times10^{1}$	51	$0.395\,062\,894\,540\,667\,149\,229\,328\,348\,029\,66\times10^{2}$
2	$0.100\,000\,000\,000\,000\,000\,000\,000\,000\,000\,00\times10^{1}$	52	$0.399\,425\,120\,952\,148\,797\,531\,222\,152\,342\,32\times10^{2}$
3	$0.350\,000\,000\,000\,000\,000\,000\,000\,000\,000\,00\times10^{1}$	53	$0.410\,060\,191\,101\,602\,090\,043\,052\,397\,782\,74\times10^{2}$
4	$0.367\,857\,142\,857\,142\,857\,142\,857\,142\,857\,14\times10^{2}$	54	$0.414\,436\,986\,960\,688\,898\,891\,492\,119\,354\,30\times10^{2}$
5	$0.511\,754\,507\,628\,294\,036\,061\,026\,352\,288\,49\times10^{1}$	55	$0.425\,057\,700\,187\,133\,663\,955\,530\,828\,596\,63\times10^{2}$
6	$0.529\,084\,738\,158\,780\,194\,674\,699\,064\,648\,39\times10^{1}$	56	$0.429\,448\,168\,737\,101\,014\,650\,144\,618\,360\,48\times10^{2}$
7	$0.656\,992\,945\,635\,443\,504\,974\,267\,757\,894\,30\times10^{1}$	57	$0.440\,055\,398\,036\,081\,358\,283\,148\,613\,748\,85\times10^{2}$
8	$0.682\,380\,046\,666\,796\,369\,997\,492\,169\,618\,18\times10^{1}$	58	$0.444\,458\,728\,894\,372\,086\,199\,596\,183\,379\,70\times10^{2}$
9	$0.805\,033\,864\,421\,748\,125\,122\,706\,818\,683\,30\times10^{1}$	59	$0.455\,053\,264\,277\,198\,102\,281\,459\,916\,718\,60\times10^{2}$
10	$0.834\,849\,779\,863\,963\,854\,923\,547\,691\,830\,07\times10^{1}$	60	$0.459\,468\,722\,351\,907\,595\,949\,580\,097\,296\,93\times10^{2}$
11	$0.953\,887\,246\,857\,987\,972\,577\,023\,231\,795\,96\times10^{1}$	61	$0.470\,051\,281\,348\,031\,118\,574\,483\,220\,537\,32\times10^{2}$
12	$0.986\,479\,549\,719\,717\,620\,914\,713\,741\,957\,99\times10^{1}$	62	$0.474\,478\,197\,506\,520\,336\,591\,765\,158\,075\,00\times10^{2}$
13	$0.110\,316\,101\,853\,427\,460\,262\,096\,418\,987\,92\times10^{2}$	63	$0.485\,049\,434\,027\,982\,991\,465\,341\,454\,063\,56\times10^{2}$
14	$0.113\,771\,506\,190\,036\,685\,988\,392\,803\,859\,67\times10^{2}$	64	$0.489\,487\,197\,193\,095\,539\,865\,145\,684\,955\,51\times10^{2}$
15	$0.125\,264\,716\,048\,108\,722\,408\,461\,301\,736\,51\times10^{2}$	65	$0.500\,047\,709\,061\,974\,229\,750\,244\,009\,758\,80\times10^{2}$
16	$0.128\,867\,402\,271\,404\,925\,792\,071\,911\,584\,66\times10^{2}$	66	$0.504\,495\,759\,477\,313\,932\,574\,232\,304\,554\,75\times10^{2}$
17	$0.140\,227\,502\,856\,243\,865\,038\,485\,649\,033\,48\times10^{2}$	67	$0.515\,046\,094\,854\,873\,138\,141\,976\,693\,696\,31\times10^{2}$
18	$0.143\,944\,698\,679\,579\,468\,163\,066\,395\,499\,11\times10^{2}$	68	$0.519\,503\,918\,314\,520\,958\,203\,730\,309\,382\,87\times10^{2}$
19	$0.155\,198\,969\,500\,280\,468\,552\,988\,656\,072\,01\times10^{2}$	69	$0.530\,044\,581\,221\,052\,513\,423\,761\,199\,539\,60\times10^{2}$
20	$0.159\,008\,772\,108\,170\,457\,082\,583\,134\,091\,17\times10^{2}$	70	$0.534\,511\,704\,101\,124\,200\,150\,311\,468\,628\,28\times10^{2}$
21	$0.170\,176\,531\,513\,355\,303\,470\,668\,676\,426\,43\times10^{2}$	71	$0.545\,043\,159\,177\,559\,707\,323\,539\,734\,178\,18\times10^{2}$
22	$0.174\,062\,844\,711\,855\,290\,912\,089\,365\,163\,91\times10^{2}$	72	$0.549\,519\,144\,138\,646\,251\,913\,826\,993\,864\,77\times10^{2}$
23	$0.185\,158\,474\,857\,522\,886\,628\,365\,932\,534\,98\times10^{2}$	73	$0.560\,041\,820\,772\,415\,204\,732\,052\,940\,899\,15\times10^{2}$
24	$0.189\,109\,270\,583\,474\,780\,611\,077\,125\,258\,00\times10^{2}$	74	$0.564\,526\,263\,026\,122\,201\,961\,906\,128\,951\,37\times10^{2}$
25	$0.200\,143\,617\,281\,603\,931\,851\,915\,593\,168\,51\times10^{2}$	75	$0.575\,040\,558\,941\,446\,817\,747\,836\,422\,306\,19\times10^{2}$
26	$0.204\,149\,682\,466\,630\,944\,991\,704\,941\,041\,23\times10^{2}$	76	$0.579\,533\,082\,993\,430\,389\,150\,059\,711\,202\,47\times10^{2}$
27	$0.215\,131\,196\,369\,972\,169\,110\,267\,287\,794\,11\times10^{2}$	77	$0.590\,039\,367\,388\,331\,944\,199\,830\,543\,378\,74\times10^{2}$
28	$0.219\,185\,248\,622\,691\,909\,765\,542\,017\,806\,67\times10^{2}$	78	$0.594\,539\,624\,185\,777\,357\,909\,453\,972\,381\,88\times10^{2}$
29	$0.230\,120\,671\,036\,695\,499\,225\,319\,895\,762\,49\times10^{2}$	79	$0.605\,038\,240\,483\,544\,501\,492\,427\,007\,954\,60\times10^{2}$
30	$0.234\,216\,854\,376\,181\,184\,389\,246\,469\,914\,06\times10^{2}$	80	$0.609\,545\,904\,907\,611\,645\,077\,964\,042\,984\,43\times10^{2}$
31	$0.245\,111\,641\,250\,767\,613\,961\,258\,724\,270\,47\times10^{2}$	81	$0.620\,037\,173\,178\,787\,358\,038\,267\,263\,874\,09\times10^{2}$
32	$0.249\,245\,176\,960\,233\,479\,119\,856\,814\,994\,64\times10^{2}$	82	$0.624\,551\,941\,832\,644\,082\,714\,661\,121\,304\,38\times10^{2}$
33	$0.260\,103\,813\,298\,516\,542\,667\,646\,000\,282\,68\times10^{2}$	83	$0.635\,036\,160\,934\,209\,519\,785\,730\,545\,728\,16\times10^{2}$
34	$0.264\,270\,740\,230\,404\,105\,837\,444\,259\,426\,93\times10^{2}$	84	$0.639\,557\,750\,185\,388\,135\,287\,435\,369\,663\,37\times10^{2}$
35	$0.275\,096\,966\,452\,121\,397\,466\,035\,445\,866\,62\times10^{2}$	85	$0.650\,035\,199\,656\,251\,043\,049\,700\,854\,319\,59\times10^{2}$
36	$0.279\,293\,958\,828\,064\,316\,518\,417\,326\,918\,48\times10^{2}$	86	$0.654\,563\,343\,898\,653\,012\,769\,105\,873\,379\,81\times10^{2}$
37	$0.290\,090\,929\,819\,401\,179\,591\,041\,170\,541\,10\times10^{2}$	87	$0.665\,034\,285\,644\,363\,384\,508\,474\,389\,124\,47\times10^{2}$
38	$0.294\,315\,166\,376\,825\,053\,017\,923\,757\,035\,30\times10^{2}$	88	$0.669\,568\,735\,750\,652\,624\,372\,948\,269\,938\,43\times10^{2}$
39	$0.305\,085\,569\,395\,378\,067\,541\,384\,292\,694\,27\times10^{2}$	89	$0.680\,033\,415\,545\,166\,393\,139\,988\,642\,893\,74\times10^{2}$
40	$0.309\,334\,633\,997\,583\,373\,032\,528\,901\,367\,33\times10^{2}$	90	$0.684\,573\,937\,484\,773\,042\,562\,964\,021\,060\,44\times10^{2}$
41	$0.320\,080\,779\,166\,108\,297\,526\,546\,399\,647\,80\times10^{2}$	91	$0.695\,032\,586\,312\,857\,882\,900\,302\,340\,362\,08\times10^{2}$
42	$0.324\,352\,584\,371\,172\,408\,967\,278\,847\,527\,99\times10^{2}$	92	$0.699\,578\,959\,914\,531\,937\,144\,755\,605\,770\,88\times10^{2}$
43	$0.335\,076\,474\,114\,153\,616\,743\,272\,510\,034\,40\times10^{2}$	93	$0.710\,031\,795\,174\,902\,033\,555\,547\,714\,992\,07\times10^{2}$
44	$0.339\,369\,202\,473\,311\,947\,430\,029\,045\,876\,00\times10^{2}$	94	$0.714\,583\,813\,015\,844\,583\,865\,502\,929\,562\,28\times10^{2}$
45	$0.350\,072\,585\,140\,770\,153\,346\,742\,890\,079\,91\times10^{2}$	95	$0.725\,031\,039\,602\,194\,416\,441\,177\,963\,645\,29\times10^{2}$
46	$0.354\,384\,643\,431\,628\,850\,574\,456\,413\,185\,64\times10^{2}$	96	$0.729\,588\,506\,008\,368\,309\,484\,071\,483\,648\,07\times10^{2}$
47	$0.365\,069\,055\,535\,766\,081\,919\,360\,183\,832\,33\times10^{2}$	97	$0.740\,030\,317\,283\,039\,195\,380\,406\,799\,280\,83\times10^{2}$
48	$0.369\,399\,038\,379\,231\,121\,257\,491\,205\,286\,41\times10^{2}$	98	$0.744\,593\,047\,427\,417\,354\,862\,368\,402\,346\,75\times10^{2}$
49	$0.380\,065\,838\,381\,361\,896\,595\,589\,998\,583\,94\times10^{2}$	99	$0.755\,029\,626\,100\,384\,391\,479\,937\,004\,560\,05\times10^{2}$
50	$0.384\,412\,498\,970\,834\,659\,472\,073\,992\,953\,38\times10^{2}$	100	$0.759\,597\,445\,187\,710\,471\,516\,055\,588\,457\,85\times10^{2}$

The first differences of the c_n for a given state, $\Delta_n^{(1)}=c_{n+1}-c_n$ (we temporarily omit the quantum-number superscripts), are observed to alternate between two sequences which converge to distinct values. This suggests that the sequence $\{c_n\}$ is composed of two subsequences $\{c_{n,\text{even}}\}$ and $\{c_{n,\text{odd}}\}$. In Table IV are listed the first and second differences of these subsequences,

$$\Delta_n^{(1)}=c_{n+2}-c_n\ ,$$
$$\Delta_n^{(2)}=c_{n+4}-2c_{n+2}+c_n\ , \tag{4.2}$$

n even and odd, for the ground-state coefficients of Table III. The observation that $\Delta_n^{(1)}\to\frac{3}{2}$ and $\Delta_n^{(2)}\to0$ for both sequences agrees with the prediction of Eq. (4.1b). Nu-

TABLE IV. The first and second differences, as defined in Eq. (4.2), of the even- and odd-indexed charmonium ground-state S-fraction coefficients c_n.

n	$\Delta_n^{(1)}$	$\Delta_n^{(2)}$	n	$\Delta_n^{(1)}$	$\Delta_n^{(2)}$
1	2.000 000 0	−0.382 454 9	2	2.678 571 4	−1.066 295 5
3	1.617 545 1	−0.165 160 7	4	1.612 276 0	−0.079 322 9
5	1.452 384 4	0.028 024 8	6	1.532 953 1	−0.008 255 8
7	1.480 409 2	0.008 124 6	8	1.524 697 3	−0.008 399 6
9	1.488 533 8	0.004 203 9	10	1.516 297 7	−0.003 942 6
11	1.492 737 7	0.002 123 7	12	1.512 355 1	−0.002 765 5
13	1.494 861 4	0.001 417 3	14	1.509 589 6	−0.001 860 0
15	1.496 278 7	0.000 868 0	16	1.507 729 6	−0.001 322 3
17	1.497 146 7	0.000 609 5	18	1.506 407 3	−0.001 000 1
19	1.497 756 2	0.000 438 1	20	1.505 407 3	−0.000 764 7
21	1.498 194 3	0.000 319 9	22	1.504 642 6	−0.000 601 4
23	1.498 514 2	0.000 243 7	24	1.504 041 2	−0.000 484 6
25	1.498 757 9	0.000 189 6	26	1.503 556 6	−0.000 396 0
27	1.498 947 5	0.000 149 6	28	1.503 160 6	−0.000 328 3
29	1.499 097 0	0.000 120 2	30	1.502 832 3	−0.000 275 9
31	1.499 217 2	0.000 098 1	32	1.502 556 3	−0.000 234 5
33	1.499 315 3	0.000 081 0	34	1.502 321 9	−0.000 201 1
35	1.499 396 3	0.000 067 6	36	1.502 120 8	−0.000 174 0
37	1.499 464 0	0.000 057 0	38	1.501 946 8	−0.000 151 7
39	1.499 521 0	0.000 048 5	40	1.501 795 0	−0.000 133 2
41	1.499 569 5	0.000 041 6	42	1.501 661 8	−0.000 117 7
43	1.499 611 1	0.000 035 9	44	1.501 544 1	−0.000 104 6
45	1.499 647 0	0.000 031 2	46	1.501 439 5	−0.000 093 4
47	1.499 678 3	0.000 027 3	48	1.501 346 1	−0.000 083 9
49	1.499 705 6	0.000 024 0	50	1.501 262 2	−0.000 075 6
51	1.499 729 7	0.000 021 3	52	1.501 186 6	−0.000 068 4
53	1.499 750 9	0.000 018 9	54	1.501 118 2	−0.000 062 2
55	1.499 769 8	0.000 016 8	56	1.501 056 0	−0.000 056 7
57	1.499 786 6	0.000 015 1	58	1.500 999 3	−0.000 051 8
59	1.499 801 7	0.000 013 6	60	1.500 947 5	−0.000 047 5
61	1.499 815 3	0.000 012 2	62	1.500 900 0	−0.000 043 7
63	1.499 827 5	0.000 011 1	64	1.500 856 2	−0.000 040 3
65	1.499 838 6	0.000 010 1	66	1.500 815 9	−0.000 037 3
67	1.499 848 6	0.000 009 2	68	1.500 778 6	−0.000 034 6
69	1.499 857 8	0.000 008 4	70	1.500 744 0	−0.000 032 1

merical agreement is also found for $N=2,3$.

At present, there exists no *a priori* expression for any terms subdominant to the linear term in Eq. (4.1b). Detailed numerical investigations indicate that for a number of perturbation problems, the next term is a constant. For the charmonium S-fraction coefficients, expansions of the form

$$c_n^{NLM}=\tfrac{3}{4}N^3n+A^{(i),NLM}+\sum_{j=1}\frac{B_j^{(i),NLM}}{[n^\alpha]^j}\ ,$$
$$i=\begin{cases}1\ , & n \text{ even}\\ 2\ , & n \text{ odd}\ ,\end{cases} \tag{4.3}$$

were assumed in an attempt to extract accurate estimates of the constants $A^{(1),NLM}$ and $A^{(2),NLM}$. Equation (4.3) represents a generalization of the expansion associated with the traditional Neville-Richardson extrapolation schemes, for which $\alpha=1$. A similar method was employed for the S-fraction representations of the quartic anharmonic oscillator.[13]

The Thiele-Padé method[44] has been the primary means of determining the constants in (4.3). Here, $[P,P]$ Padé approximants of the form

$$c_n-\tfrac{3}{4}N^3n=\frac{p_0^{(i)}+p_1^{(i)}z+\cdots+p_p^{(i)}z^P}{1+q_1^{(i)}z+\cdots+q_P^{(i)}z^P}\ ,$$
$$i=\begin{cases}1\ , & n \text{ even}\\ 2\ , & n \text{ odd}\ ,\end{cases} \tag{4.4}$$

where $z=n^{-\alpha}$, $\alpha>0$, are constructed from a set of $2P+1$ points (usually, for convenience in programming, the consecutive points $c_r,c_{r+2},\ldots,c_{r+4P}$) by a continued-fraction algorithm. Evaluation of the Padé approximant at $z=0$, corresponding to $n=\infty$, gives

$$p_0^{(i)}\cong A^{(i)}\ ,\quad i=1,2\ . \tag{4.5}$$

By varying r and P, an idea of the accuracy as well as the stability of the fitting procedure should be obtained.

For $\alpha=1$ in (4.3), both Neville-Richardson and Thiele-

Padé schemes yield estimates of disappointing accuracy. Using ground-state coefficients c_n even to $n=105$, we find $A^{(1)}=0.26\pm0.02$, $A^{(2)}=-0.24\pm0.02$. Moreover, when the parameter α is varied, the $A^{(i)}$ also vary. Interestingly enough, the difference $\Delta A=A^{(1)}-A^{(2)}$ is preserved as α varies, to roughly two digits. However, for the case $\alpha=\frac{1}{2}$, both extrapolation schemes stabilize and consistently yield (for various values of P and r) $A^{(1)}=1$ and $A^{(2)}=\frac{5}{4}$ to less than one part in 10^5 for the ground-state representation. (A stabilization at $\alpha=\frac{1}{2}$ was also observed in Ref. 13.) Analysis of excited-state representations reveals a regular behavior in the constants, independent of the angular quantum number L: $A^{(1),NLM}=N^3(-\frac{1}{2}+\frac{3}{2}N)$, $A^{(2),NLM}=N^3(-\frac{1}{4}+\frac{3}{2}N)$. The L independence is seen in the numerical behavior of the c_n^{NLM}. The even and odd sequences of $\{c_n^{200}\}$ and $\{c_n^{210}\}$ have approached each other quite closely at $n\sim90$, as is also observed for those of $\{c_n^{300}\}$, $\{c_n^{310}\}$, and $\{c_n^{320}\}$.

On the basis of this numerical evidence, the following asymptotic behavior is conjectured for the charmonium S-fraction coefficients:

$$c_{n,\text{even}}^{NLM}\sim\tfrac{3}{4}N^3(n+2N)-\tfrac{1}{2}N^3+R_n^{(1),NLM}\ \text{as}\ n\to\infty\ ,$$
$$c_{n,\text{odd}}\sim\tfrac{3}{4}N^3(n+2N)-\tfrac{1}{4}N^3+R_n^{(2),NLM}\ \text{as}\ n\to\infty\ , \tag{4.6}$$

where $R_n^{(i)}=o(1)$. The charmonium CF representations are $S_{(1)}$ fractions. By Eq. (C10) of Appendix C, these fractions converge uniformly in $E_{NLM}(\lambda)$ on compact subsets of the cut plane $|\arg\lambda|<\pi$. This is (necessarily) consistent with the remarks on Padé summability made at the end of Sec. III.

From a computational viewpoint, a knowledge of $S_{(k)}$-fraction asymptotics for $k=1,2$ has been shown useful[11] in the estimation of energy eigenvalues $E(\lambda)$ for rather large values of the coupling constant λ. In the case of $S_{(1)}$-fraction representations, Thiele-Padé extrapolation of a small number of accurately known c_n produces an approximate "tail" of $C(\lambda)$ which affords good estimates of $E(\lambda)$. Of course, due to the relative simplicity of Eq. (1.1), vastly superior methods of obtaining its eigenvalues exist, e.g., numerical integration. As such, no further computational aspects of this problem will be discussed.

Several aspects of $S_{(1)}$-fraction asymptotics are most interesting from an analytic viewpoint, revealing additional intimate relationships between a CF and its corresponding perturbation series as well as between the CF and the function $E(\lambda)$. We postpone a detailed discussion of these aspects for a future paper,[45] but outline below some interesting features which are relevant to the charmonium problem.

First, let us consider the generalized Euler series,

$$\bar{E}(\lambda)=1+A\sum_{n=1}^{\infty}(-1)^{n+1}\Gamma(n+\alpha)k^nz^n\ , \tag{4.7}$$

where A, α, and k are constants, and its CF representation,

$$\bar{E}(\lambda)=1+\cfrac{\bar{c}_1}{1+\cfrac{\bar{c}_2}{1+\cfrac{\bar{c}_3}{1+\cdots}}}\ . \tag{4.8}$$

The $S_{(1)}$-fraction coefficients $\bar{c}_n$ are easily determined from a look at the QD table associated with (4.7):

$$\bar{c}_1=kA\Gamma(1+\alpha)\ ,$$
$$\bar{c}_{n,\text{even}}=\frac{k}{2}+k\alpha\ , \tag{4.9}$$
$$\bar{c}_{n,\text{odd}}=\frac{k}{2}n+\frac{k}{2}\ .$$

Now consider the generalized Euler series $\bar{E}_{NLM}(\lambda)$ whose coefficients are composed of the leading terms of the charmonium RS perturbation coefficients in (3.25). In this case, $\alpha=2N$, $k=\frac{3}{2}N^3$. The coefficients of its $S_{(1)}$-fraction representation are given by

$$\bar{c}_1=\tfrac{3}{2}N^3A\Gamma(2N+1)\ ,$$
$$\bar{c}_{n,\text{even}}=\tfrac{3}{4}N^3(n+4N)\ , \tag{4.10}$$
$$\bar{c}_{n,\text{odd}}=\tfrac{3}{4}N^3(n-1)\ ,\quad n>2$$

where A represents the constant in (3.25). A look at (4.6) and (4.10) reveals the interesting set of relations

$$c_{n,\text{even}}=\bar{c}_{n,\text{even}}-k\epsilon_N+R_n^{(1),NLM}\ ,$$
$$c_{n,\text{odd}}=\bar{c}_{n,\text{odd}}+k\epsilon_N+R_n^{(2),\text{NLM}}\ , \tag{4.11}$$

where $\epsilon_N=N+\frac{1}{3}$. In other words, the true charmonium coefficients c_n^{NLM} are, to order $O(1)$, obtained from the hypergeometric coefficients $\bar{c}_n^{NLM}$ by an alternating perturbation $(-1)^{n+1}k\epsilon_N$, $n\geq2$. One may consider the perturbation to be induced by the asymptotic corrections (3.26) to the LOPT formula (3.25). This mechanism is partially understood and will be discussed elsewhere.

A second important feature of the charmonium $S_{(1)}$ fractions is the *asymptotic phase shift* of their coefficients c_n^{NLM} in (3.6), which we define as

$$\Delta A=A^{(1),NLM}-A^{(2),NLM}=-\tfrac{1}{4}N^3\ . \tag{4.12}$$

It will be shown in another paper that this quantity is related to the high-field limit of Eq. (2.3), specifically,

$$E_{NLM}(\lambda)\sim F_{NLM}^{(0)}\lambda^{1/2-\Delta A/k}\ \text{as}\ \lambda\to\infty\ , \tag{4.13}$$

where, as before, $k=\frac{3}{4}N^3$. This result is in accordance with the results of Appendix B. Moreover, the $S_{(1)}$-fraction representations yield accurate estimates of the leading coefficients $F_{NLM}^{(0)}$.

V. CONCLUDING REMARKS

The so(4,2) Lie-algebraic reformulation described in Sec. II may easily be extended to treat generalized charmonium potentials of the form

$$-\tfrac{1}{2}\nabla^2-\frac{Z}{r}+\lambda r^p,\quad p=2,3,4,\ldots\ . \tag{5.1}$$

The perturbation λr^p may also be replaced by a polynomial in λ and r. Specific polynomial perturbations have received interest.[46,47] The algebraically reformulated version of (5.1) is simply

$$\left[(\hat{T}_3-N)+\lambda\left[\frac{N}{Z}\right]^{p+2}(\hat{T}_3-\hat{T}_1)^{p+1}+\Delta E\left[\frac{N}{Z}\right]^2(\hat{T}_3-\hat{T}_1)\right]\psi=0\ . \quad (5.2)$$

The matrix elements of the operator $(\hat{T}_3-\hat{T}_1)^{p+1}$ may be determined analytically by iteration of Eq. (2.15) or numerically by brute-force matrix multiplication. From Eq. (2.15) it is easily seen that its matrix representation is $(2p+3)$-diagonal in a fixed-(L,M) subspace.

The Bender-Wu LOPT formulas of Eq. (5.1) for $p=2$, corresponding to a spherically symmetric version of the quadratic Zeeman effect in hydrogen, have also been determined.[32] The RS perturbation expansions are $\Gamma(2n)$-type Stieltjes series. An analysis of the general case $p\geq 1$, to be published elsewhere, shows that $E^{(n)}\sim(-1)^{n+1}\Gamma(pn)$. From Carleman's theorem, the moment problem is guaranteed determinate for $p=1,2$. The CF representations of these generalized charmonium expansions are expected to be $S_{(p)}$ fractions. This has been observed numerically for the case $p=2$. The ground-state S-fraction coefficients behave as $c_n\sim 2n^2$, $n\rightarrow\infty$.

An asymptotic analysis of S-fraction coefficients corresponding to $\Gamma(pn)$-type Stieltjes series is severely limited due to the nonlinear nature of the QD algorithm. The $S_{(1)}$ asymptotic formulas conjectured in Eqs. (4.6) are, beyond the dominant terms, based on numerical evidence. The superior extrapolation afforded by an expansion of the form (4.3) for $\alpha=\frac{1}{2}$ still remains an enigma. However, the $S_{(1)}$ asymptotic phase shifts, Eq. (4.12), deduced from this numerical evidence correctly accounts for the high-field limit, Eq. (4.13), for a number of perturbation problems as will be shown elsewhere.

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APPENDIX A: HYDROGENIC RSPT BY DIFFERENCE EQUATIONS

We briefly outline a difference-equation technique which is analogous to a method employed for the study of anharmonic oscillators.[48] Such an approach to the quadratic Zeeman effect in hydrogen, which is more complicated, was outlined in an earlier paper.[11]

One basically assumes a Frobenius-type solution to the modified eigenvalue problem, Eq. (2.5). The complete and discrete set of so(4,2) Sturmian basis functions $\chi_{nlm}(\mathbf{r})$ share a common exponential factor e^{-r} unlike their hydrogenic counterparts $\psi_{nlm}(\mathbf{r})$, cf. Eq. (2.14). This makes it possible to assume a solution of the form

$$\psi=e^{-r}B(r)Y_{LM}(\theta,\phi)\ , \quad (A1)$$

where

$$B(r)=\sum_{n=0}^{\infty}\lambda^n B_n(r)\ , \quad (A2)$$

$$B_n(r)=\sum_j b_{jn}r^j\ . \quad (A3)$$

This method is compact and may easily be adapted for rational arithmetic calculations. A drawback, however, is that the difference equation must be reformulated for each particular state concerned, since it is dependent upon the structure of the unperturbed solution.

For the ground state, for example, we have the initial condition

$$B_0(r)=b_{00}=1\ . \quad (A4)$$

Substitution of Eqs. (A1)—(A4) into Eq. (2.7) eventually yields the following difference equation for the b_{jn}:

$$b_{jn}=\frac{1}{2j}(j+1)(j+2)b_{j+1,n}-\frac{1}{j}b_{j-2,n-1}-\frac{3}{j}\sum_{i=1}^{n-1}b_{2,i}b_{j-1,n-i},\quad n=1,2,3,\ldots \quad (A5)$$

where $b_{j,0}=0$ for $j>0$, $b_{1,n}=0$ for $n>0$, and $b_{jn}=0$ if $j>n$. The perturbation coefficients $E^{(n)}_{NLM}$ are given by

$$E^{(n)}=-3b_{2,n}\ . \quad (A6)$$

This difference-equation approach may easily be extended to treat higher-order radial perturbations of the hydrogen atom where $\hat{V}=\lambda r^p$, $p=2,3,\ldots$ or where r^p is replaced by a polynomial in r.

APPENDIX B: THE HIGH-FIELD LIMIT FOR CHARMONIUM

In this appendix, we outline a Symanzik-type scaling transformation of the eigenvalue problem,

$$(-\tfrac{1}{2}\nabla^2-Z/r+\lambda r)\psi=E(\lambda)\psi \quad (B1)$$

(Z constant), to elucidate the high-field asymptotics of $E(\lambda)$ as $\lambda\rightarrow\infty$. First, set $\mathbf{r}=\alpha\mathbf{r}'$ where α is a real parameter, and drop the primes to give

$$\left[-\tfrac{1}{2}\nabla^2-\frac{Z\alpha}{r}+\lambda\alpha^3 r\right]\psi=\alpha^2E(\lambda)\psi\ . \quad (B2)$$

Now let $\alpha=\lambda^{-1/3}$ and rewrite (B2) as

$$\left[-\tfrac{1}{2}\nabla^2+r-\frac{\beta}{r}\right]\psi=F(\beta)\psi\ , \quad (B3)$$

where $\beta=Z\lambda^{-1/3}$ and $F(\beta)=\lambda^{-2/3}E(\lambda)$. Clearly, $\beta\rightarrow 0$ as $\lambda\rightarrow\infty$.

The "unperturbed" problem corresponding to Eq. (B3), representing the infinite field limit for (B1), is a three-dimensional Airy eigenvalue equation

$$(-\tfrac{1}{2}\nabla^2+r)\phi=F^{(0)}\phi\ . \tag{B4}$$

Its solutions have the usual form

$$\phi_{plm}(\mathbf{r})=\frac{1}{r}T_{pl}(r)Y_{lm}(\theta,\phi)\ , \tag{B5}$$

where the radial functions $T_{pl}(r)$ satisfy

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{1}{2}\frac{l(l+1)}{r^2}+r-F^{(0)}\right]T_{pl}(r)=0 \tag{B6}$$

and behave as $T_{pl}(r)\sim c_{pl}r^{l+1}$ as $r\to 0$ for c_{pl} constant. A correspondence between low-field states ψ_{nlm} and high-field states ϕ_{plm} may be made by an "*Aufbau*-like" procedure where l and m remain fixed and the number of nodes in the radial functions R_{nl} and T_{pl} are compared.[3]

It is convenient to "unscale" Eq. (B6) by setting $r=2^{1/3}r'$, and again dropping primes to yield

$$\left[-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}+r-\bar{F}^{(0)}\right]y(r)=0\ , \tag{B7}$$

where $\bar{F}^{(0)}=2^{1/3}F^{(0)}$. The "physical" solutions of (B7) obey the boundary conditions $y(0)=0$, $y(r)\to 0$ as $r\to\infty$. For $l=0$, the eigenfunctions of (B7) are given by the standard Airy functions[49]

$$y=\mathrm{Ai}(r-\bar{F}^{(0)})\ . \tag{B8}$$

The energy eigenvalues of (B7) for $l=0$ are given by the zeros of the Airy function,

$$\mathrm{Ai}(-\bar{F}^{(0)})=0\ . \tag{B9}$$

For $l\neq 0$, the eigenvalues and eigenfunctions of (B7) must be calculated numerically. Eichten *et al.*[3] have calculated the eigenvalues of the seven lowest-lying states.

The perturbation problem in (B3) suggests an eigenvalue expansion of the form

$$F(\beta)=F^{(0)}+\sum_{k=1}^{\infty}F^{(k)}\beta^k \text{ as } \beta\to 0\ . \tag{B10}$$

From Eq. (B2), this would imply the following asymptotic expansion for $E(\lambda)$:

$$E(\lambda)=F^{(0)}\lambda^{2/3}+\sum_{k=1}^{\infty}G^{(k)}\lambda^{(2-n)/3} \text{ as } \lambda\to\infty\ , \tag{B11}$$

where $G^{(k)}=Z^kF^{(k)}$.

APPENDIX C: SOME IMPORTANT PROPERTIES OF CONTINUED FRACTIONS

Continued fractions play an important role in a wide variety of mathematical disciplines ranging from number theory to combinatorics. Along with this diverse applicability, a number of special types of continued-fraction functions of a complex variable may be formulated. This appendix outlines the important properties of a special type of continued fraction which is well suited for the representation of perturbation series. For a comprehensive and very readable presentation of analytic theory of continued fractions, the book by Jones and Thron[50] is strongly recommended. We also mention the classic treatises of Wall[51] and Perron.[52] Details of the material presented below may be found in the above mentioned references as well as in the book of Henrici[33] and the standard references on Padé approximants.[44,53]

A RITZ continued fraction[33] is defined as the following function of a complex variable $z\in\mathbb{C}$:

$$C(z)=\cfrac{c_1}{1+\cfrac{c_2z}{1+\cfrac{c_3z}{1+\cdots}}} \tag{C1}$$

which may be expressed in a more typographically convenient form as

$$C(z)=\frac{c_1}{1+}\,\frac{c_2z}{1+}\,\frac{c_3z}{1+}\cdots\ . \tag{C2}$$

If we set $c_{n+1}=0$ then (C2) reduces to a finite or truncated fraction,

$$w_n(z)=\frac{c_1}{1+}\,\frac{c_2z}{1+}\cdots\frac{c_nz}{+1}\ , \tag{C3}$$

the nth approximant of $C(z)$, which may be expressed as a rational function. The numerators and denominators of these approximants obey the recurrence relations

$$w_n(z)=\frac{A_n(z)}{B_n(z)}=\frac{A_{n-1}(z)+zc_nA_{n-2}(z)}{B_{n-1}(z)+zc_nB_{n-2}(z)}\ , \tag{C4}$$

with initial values $A_0=0$, $B_0=1$, $A_1=c_1$, $B_1=1$. Moreover,

$$\deg[A_n(z)]=\left[\frac{n-1}{2}\right]$$

and

$$\deg[B_n(z)]=\left[\frac{n}{2}\right]\ ,$$

where $[x]$ denotes "the greatest integer contained in x." $C(z)$ is said to converge at a point z_0 if $\lim_{n\to\infty}w_n(z_0)$ exists and is finite. The region of convergence of $C(z)$ is the set of all $z\in\mathbb{C}$ for which $C(z)$ converges.

The continued fraction $C(z)$ in (C2) is said to be *equivalent* to the formal power series (whether or not the series is convergent),

$$f(z)=\sum_{n=0}^{\infty}a_nz^n\ , \tag{C5}$$

if the Taylor-series expansion of its nth convergent $w_n(z)$ agrees with $f(z)$ to the term a_nz^n for all n, i.e., if

$$w_n(z)-f(z)=O(z^{n+1})\ ,\quad n=0,1,2,\ldots\ . \tag{C6}$$

Thus $w_{2N}(z)$ and $w_{2N+1}(z)$ are, respectively, the $[N-1,N]$ and $[N,N]$ Padé approximants to $f(z)$. The sequence $w_n(z)$ generates a stepwise descent of the Padé table of $f(z)$.

The existence and uniqueness of a RITZ CF representation to a formal power series is ensured if $f(z)$ is normal, i.e., if the Hankel determinants of the series, defined by

$$H_k^{(n)}=\begin{vmatrix} a_n & a_{n+1} & \cdots & a_{n+k-1} \\ a_{n+1} & a_{n+2} & \cdots & a_{n+k} \\ \vdots & \vdots & & \vdots \\ a_{n+k-1} & a_{n+k} & \cdots & a_{n+2k-2} \end{vmatrix}, \tag{C7}$$

satisfy $H_k^{(n)}\neq 0$, $n=0,1$ and $k=1,2,3,\ldots$.

Of particular importance to this study are CF representations of Stieltjes series—series whose coefficients a_n may be expressed in terms of the moments of a nonnegative distribution $\psi(t)$ having infinitely many points of increase on the positive real axis, i.e., $a_n=(-1)^n\mu_n$ where

$$\mu_n=\int_0^\infty t^n d\psi(t)\ , \quad n=0,1,2,3,\ldots \tag{C8}$$

and the integral is, in general, a Stieltjes integral. In this case, $c_n>0$, $n=1,2,3,\ldots$ and $C(z)$ is called an S fraction. The poles of all approximants $w_n(z)$ of an S fraction lie on the negative real axis. Conversely, if $C(z)$ is an S fraction, the formal power series which corresponds to it is Stieltjes. On the positive real axis, the even and odd convergents of an S fraction satisfy the bounding relations

$$w_{2N}(x)=[N-1,N]<f(x)<[N,N]=w_{2N+1}(x)\ , \quad N=0,1,2,\ldots . \tag{C9}$$

The uniqueness of the distribution $\psi(t)$ which generates the moments μ_n is not guaranteed. The S fraction may diverge, with different subsequences of the $w_n(z)$ converging to different functions. Two of these distinct functions will admit the same series as an asymptotic expansion for $z\to 0$ through positive values. The determinancy of this moment problem boils down to the convergence of the S fraction $C(z)$. A number of theorems on convergence exist. An important theorem guarantees that if

$$\sum_{n=1}^{\infty} c_n^{-1/2}=\infty\ , \tag{C10}$$

then the S fraction converges uniformly on all compact subsets of the cut plane $|\arg z|<\pi$ to a unique function $f(z)$. This guarantees that the even and odd convergents in (C9) provide lower and upper bounds which converge to $f(z)$ as $N\to\infty$.

Perhaps the most famous and useful theorem in the context of large-order perturbation theory is Carleman's theorem, stating that a sufficient condition for the convergence of $C(z)$, hence the determinacy of the moment problem, is

$$\sum_{n=1}^{\infty} \mu_n^{-1/2n}=\infty\ . \tag{C11}$$

There exist a number of algorithms to determine the CF representation of a formal power series, including the quotient-difference,[54,55] corresponding series[56] (CS), and product-difference[57] algorithms. The QD scheme, perhaps the best-known algorithm, was employed in the calculations of this report. For the power series in (C5), the QD algorithm defines the two-dimensional sequences $e_m^{(n)}$ and $q_m^{(n)}$ by the initial values

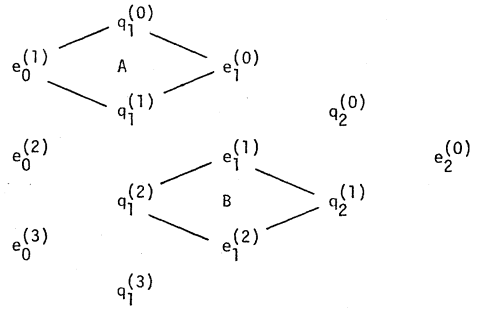

FIG. 2. The QD table, illustrating two particular unit rhombi which satisfy Eqs. (C13). For a particular power series, the first two columns of the array are initialized according to Eqs. (C12). In the forward QD algorithm, the rightmost element of each rhombus is calculated from the other three elements. A knowledge of N elements in the column $q_1^{(n)}$ determines N entries of the upper edge of the array which, by Eq. (C14), define the continued-fraction representation of the power series.

$$\begin{aligned} &e_0^{(n)}=0\ , \quad n=1,2,3,\ldots , \\ &q_1^{(n)}=-\frac{a_{n+1}}{a_n}\ , \quad n=0,1,2,\ldots , \end{aligned} \tag{C12}$$

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

$$\begin{aligned} &e_m^{(n)}=q_m^{(n+1)}-q_m^{(n)}+e_{m-1}^{(n+1)}\ , \\ &q_{m+1}^{(n)}=\frac{e_m^{(n+1)}}{e_m^{(n)}}q_m^{(n+1)}\ , \end{aligned} \tag{C13}$$

$$m=1,2,3,\ldots , \quad n=0,1,2,\ldots .$$

These sequences are traditionally presented as a set of interwoven arrays known as the QD table, shown schematically in Fig. 2. Any four elements of the table which form a unit rhombus are connected by the recursion relations of (C13).

If the power series $f(z)$ is normal, then its QD table exists and its CF representation is given by

$$C(z)=\frac{a_0}{1+}\,\frac{q_1^{(0)}z}{1+}\,\frac{e_1^{(0)}z}{1+}\,\frac{q_2^{(0)}z}{1+}\,\frac{e_2^{(0)}z}{1+}\cdots\ . \tag{C14}$$

In the *forward QD algorithm*, the first and second columns of the QD table are initialized according to Eqs. (C12). Equations (C13) are then used to calculate a QD triangle as in Fig. 2. The elements of the upper edge of this triangle, the "diagonal" entries of the array, are the elements of $C(z)$ in (C14). Each additional series coefficient a_n allows the determination of an additional RITZ fraction coefficient c_n. In this way, a one-to-one correspondence is seen to exist between the a_n and the c_n. If $f(z)$ is a series of Stieltjes, then it may be shown that all c_n are positive.

*Present address: School of Mathematics, Georgia Institute of Technology, Atlanta, GA 30332.
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