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# Nonlinear "self-interaction" Hamiltonians of the form $H^{(0)} + \lambda \langle r^p \rangle r^q$ and their Rayleigh–Schrödinger perturbation expansions

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Rayleigh–Schrödinger perturbation expansions for eigenvalues  $E(\lambda)$  of nonlinear Hamiltonians of the form  $\hat{H}^{(0)} + \lambda \langle r^p \rangle r^q$ ,  $p, q \geq 1$  are calculated using hypervirial (HV) and Hellmann–Feynman (HF) theorems. Such Hamiltonians are similar in form to those employed in the study of "self-interacting" systems, e.g., solute–solvent interactions. The specific cases considered for  $H^{(0)}$  are one-dimensional harmonic oscillators and hydrogen atoms. The eigenvalue expansions for the nonlinear problems are compared with those of the linear problems where  $p = 0$ , whose large-order behavior and summability properties are well-known. Also examined are the perturbation expansions for the expectation values  $\langle r^k \rangle$ , which are also products of the HVHF method.

## I. INTRODUCTION

Nonlinear Schrödinger equations with the generic form

$$[\hat{H}^{(0)} + \hat{V}(\psi)]\psi = E\psi \quad (1.1)$$

have been used to describe quantum mechanical systems that interact with their environment.<sup>1,2</sup> Through its wave function  $\psi$ , the system interacts with its surroundings by, for example, inducing a net field which then acts back on the system itself. This "self-dependent" situation could be described by appropriate choice of the interaction operator  $\hat{V}$  in (1.1). The linear Schrödinger equation,

$$\hat{H}^{(0)}\psi^{(0)} = E^{(0)}\psi^{(0)}, \quad (1.2)$$

is assumed to describe the system *in vacuo*, i.e., isolated and independent of its environment.

Such treatments have been employed in the studies of molecules immersed in polar solvents, a problem of prime importance in the study of biological systems. An electronic state of the molecule, described by a wave function  $\psi$ , induces an energetically favorable orientation of polar solvent molecules (e.g., water molecules) that surround it. This orientation produces a field that, in turn, acts on the molecule in question. The Hamiltonians used to describe such systems have assumed the form

$$[H^{(0)} + \lambda \langle \psi | \hat{A} | \psi \rangle \hat{B}] \psi = E(\lambda) \psi. \quad (1.3)$$

Again, the linear Schrödinger eigenvalue equation in (1.2) is usually assumed to describe the solute molecule *in vacuo*. Using the Kirkwood–Onsager model,<sup>3</sup>  $\hat{A} = \hat{B} = \hat{M}$ , the dipole moment operator. The perturbation parameter  $\lambda$  could describe the strength of the solute–solvent interaction. A variety of methods have been used to approximate the solutions of (1.3). Of course, even in the case of atoms or small molecules, the solution of (1.2) may be a formidable task.

This report was motivated by the paper of Surjan and Angyan<sup>2</sup> in which was developed a formal nondegenerate Rayleigh–Schrödinger (RS) perturbation theory for problems of the form in Eq. (1.3), assuming the solvability of the unperturbed problem in Eq. (1.2). The presence of the self-interaction introduces nonlinear contributions to the perturbation corrections to  $E$  and  $\psi$ . In the special case  $\hat{A} = \hat{1}$ , the

identity operator, the perturbation formulas reduce to the usual Rayleigh–Schrödinger perturbation theory (RSPT). In principle, the method may be used to calculate perturbation corrections to arbitrary order.

Here, we examine eigenvalue perturbation expansions for simple radial oscillators, defined by the Hamiltonians

$$\hat{H}^{(p,q)} = \frac{1}{2} \hat{p}^2 + \frac{1}{2} r^2 + \lambda \langle r^p \rangle r^q, \quad p, q = 1, 2, 3, \dots, \quad (1.4)$$

where  $\langle r^{2k} \rangle$  denotes the expectation value

$$\langle r^{2k} \rangle \equiv \frac{\int \psi^*(r) r^{2k} \psi(r) dr}{\int \psi^*(r) \psi(r) dr}, \quad (1.5)$$

$\psi$  being an eigenstate of  $\hat{H}^{(p,q)}$ . Equation (1.4) can be considered to define such oscillators in arbitrary space dimensions, but the present analysis is restricted to one-dimensional problems. The eigenvalue expansions will assume the usual form of RSPT, i.e.,

$$E_K^{(p,q)}(\lambda) = \sum_{n=0}^{\infty} E_K^{(p,q)(n)} \lambda^n, \quad (1.6)$$

where  $E_K^{(0)} = K + \frac{1}{2}$ . Their behavior will be related to that of the well-known expansions associated with the "linear" perturbation problems where  $p = 0$ , which correspond to the anharmonic oscillators studied in the context of quantum field theory.<sup>4–9</sup> In the spirit of our introductory remarks, the Hamiltonians in (1.4) could be viewed as defining self-interacting oscillators whose anharmonicities are directly proportional to the mean values of given powers of their vibrational amplitudes.

Specifically, we examine the large-order behavior of the RS coefficients  $E_K^{(p,q)(n)}$ . With the aid of numerical computations, the summability of these series is also conjectured. The coefficients are easily calculated by a method originally developed by Swenson and Danforth<sup>10</sup> to study perturbed oscillator problems. Their method, which employed the hypervirial (HV) and Hellmann–Feynman (HF) theorems, and which will henceforth be referred to as the HVHF method, permits a calculation of the (nondegenerate) eigenvalue series without a knowledge of wave functions. In short, no

matrix elements are needed and the only input into the algorithm is the unperturbed energy  $E_K(0) = E_K^{(0)}$ . A by-product of this approach is that it yields formal perturbation expansions for the expectation values  $\langle r^k \rangle$ . The HVHF method is reviewed for general  $N$ -dimensional problems in Sec. II. Section III is devoted to its application to oscillator problems. In addition to the eigenvalue expansions, the perturbation series for  $\langle r^k \rangle$  will be examined in detail for the linear eigenvalue problems. These series also possess interesting large-order and summability properties which are useful for an understanding of the nonlinear expansions.

The HVHF perturbative method has been applied to hydrogenic problems by Killingbeck<sup>11</sup> and a number of other workers, e.g., Refs. 12–15. In these problems, the traditional difficulties posed by the continuum spectrum of the unperturbed hydrogen Hamiltonian operator are bypassed. In Sec. IV, the HVHF method is applied to the following nonlinear hydrogenic counterparts:

$$\hat{H} = \frac{1}{2} \hat{p}^2 - Z/r + \lambda \langle r^p \rangle r^q, \quad p, q = 1, 2, 3, \dots \quad (1.7)$$

For both oscillator and hydrogenic cases, the nonlinear expansions will be shown to be intimately related to the corresponding expansions for the linear problems, i.e., where  $p = 0$ . In Sec. V we apply a “renormalization method” to the RS series in Eq. (1.6) to accurately calculate  $E(\lambda)$  for the entire infinite range of coupling constant values  $0 < \lambda < \infty$ . In addition, the eigenvalues of the infinite-field Hamiltonians

$$\hat{H}_{\infty}^{(p,q)} = \frac{1}{2} \hat{p}^2 + \langle r^{2p} \rangle r^{2q} \quad (1.8)$$

are calculated from the renormalized perturbation series.

## II. HYPERVIRIAL AND HELLMANN-FEYNMAN (HVHF) THEOREMS AND PERTURBATION THEORY AT LARGE ORDER

In this section, we outline the essential aspects of the HVHF method as applied to  $N$ -space-dimensional eigenvalue equations of the form

$$\hat{H}\psi_n = (\hat{T} + \hat{V})\psi_n = E_n\psi_n, \quad (2.1)$$

where  $\hat{T}$  is the kinetic energy operator and  $\hat{V} = V(r)$  is the spherically symmetric potential energy operator. Since the method is relatively well-known and has been applied by many researchers, the following description is brief. The reader is referred to a new monograph on the subject by Fernandez and Castro.<sup>16</sup> The comprehensive review article by Marc and McMillan<sup>17</sup> is also recommended for a discussion of the virial theorem and its applications in both classical and quantum mechanics.

The case of radial potentials  $\hat{V} = V(r)$  represents a relatively simple set of eigenvalue problems. A separation-of-variables approach, i.e., assuming  $\psi(r) = R(r)Y(\Omega)$ , factors out the angular  $\Omega$  dependence in terms of  $N$ -dimensional spherical harmonics. The result is the radial eigenvalue equation<sup>18</sup>

$$\hat{H}R_{nl}(r) = [\frac{1}{2}\hat{p}_r^2 + L^2/2r^2]R_{nl}(r) = E_n R_{nl}(r), \quad (2.2)$$

where the operator

$$\hat{p}_r^2 = -[\hat{D}^2 + ((N-1)/r)\hat{D}]$$

is the square of the radial momentum operator in  $N$ -dimensional space, with  $\hat{D} \equiv d/dr$ . The indices  $n$  and  $l$  represent the radial and (one of the) angular momentum quantum numbers, respectively. The scalar  $L^2 = l(l+N-2)$  represents the eigenvalue of the square of the  $N$ -dimensional angular momentum operator  $\hat{L}^2$ .

Now, given any linear operator  $\hat{Q}$ , the following expectation values vanish ( $[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$ ):

$$\langle [\hat{Q}, \hat{H}] \rangle \equiv \int \psi^*(r) [\hat{Q}, \hat{H}] \psi(r) dr = 0, \quad (2.3)$$

for all eigenstates  $\psi_n$  of  $\hat{H}$ , by virtue of the self-adjointness of  $\hat{H}$ . The wave function  $\psi$  is always assumed to be normalized to unity. If we choose  $\hat{Q} = r^k \hat{D}$  and evaluate explicitly the commutator in Eq. (2.3), a set of recursion relations involving the expectation values,  $\langle r^k \rangle \equiv \int \psi^* r^k \psi dr$ , are obtained. These equations are known as the *hypervirial relations*.<sup>19</sup> In order to evaluate the commutators, we begin with the following relations, which are easily derived from Eq. (2.2):

$$[\hat{D}, \hat{H}] = (\hat{D}V) + ((N-1)/2r^2)\hat{D} - L^2/r^3, \quad (2.4)$$

$$[r^k, \hat{H}] = kr^{k-1}\hat{D} + \frac{1}{2}k(k+N-2)r^{k-2}, \quad (2.5)$$

where  $(\hat{D}V) \equiv dV/dr$ .

The operator identity  $[r^k \hat{D}, \hat{H}] = r^k [\hat{D}, \hat{H}] + [r^k, \hat{H}] \hat{D}$  is now used to rewrite the commutator in Eq. (2.3). Any appearance of  $\hat{D}$  and  $\hat{D}^2$  is then eliminated with the use of Eqs. (2.4) and (2.5). Taking expectation values with respect to the eigenstate  $\psi_n$  yields the following hypervirial relations for an arbitrary radial potential  $V(r)$ :

$$\begin{aligned} 2kE \langle r^{k-1} \rangle &= \langle r^k (\hat{D}V) \rangle + 2k \langle r^{k-1} V \rangle + (k-1)L^2 \langle r^{k-3} \rangle \\ &\quad - \frac{1}{4}(k+N-3)[k(k-N)+N-1] \langle r^{k-3} \rangle, \\ k &= \dots, -2, -1, 0, 1, 2, \dots \end{aligned} \quad (2.6)$$

The case  $k = 1$  corresponds to the quantum mechanical virial theorem.<sup>20</sup> Since  $V(r)$  will generally be a sum of powers of  $r$ , Eq. (2.6) will imply a recurrence relation between expectation values  $\langle r^k \rangle$ . Moreover, for perturbation problems,  $V(r)$  will include the coupling constant  $\lambda$ . The essence of the HVHF perturbative method is to assume the following expansions for a given state in question:

$$E = \sum_{n=0}^{\infty} E^{(n)} \lambda^n, \quad (2.7)$$

$$\langle r^k \rangle = \sum_{n=0}^{\infty} C_k^{(n)} \lambda^n. \quad (2.8)$$

It is assumed that the unperturbed energy  $E^{(0)}$  is known. Also, the normalization condition  $\langle r^0 \rangle = 1$  is imposed, implying that

$$C_0^{(n)} = \delta_{0n}. \quad (2.9)$$

Substitution of these expansions into Eq. (2.6) and collection of like powers of  $\lambda^n$  yield a difference equation in the coefficients  $C_i^{(n)}$  and  $E^{(k)}$ . An application of the Hellmann-Feynman theorem,<sup>21</sup>

$$\frac{dE}{d\lambda} = \left\langle \frac{\partial H}{\partial \lambda} \right\rangle = \sum_{n=0}^{\infty} (n+1) E^{(n+1)} \lambda^n, \quad (2.10)$$

defines the relation between the  $E^{(k)}$  and the  $C_i^{(j)}$ . General-

ly, the  $C_i^{(j)}$  array is calculated "columnwise," starting from the  $n = 0$  (unperturbed) column, whose elements are computed recursively. The triangular nature of this computation will be seen in the examples that follow.

In traditional "textbook" presentations of Rayleigh-Schrödinger perturbation theory, little attention is paid to questions concerning the nature of the expansions obtained. Usually, it is naively assumed that for sufficiently small  $\lambda$  the series converges. Of course, these questions were addressed many years ago<sup>22</sup> and have continued to receive attention. Many eigenvalue expansions encountered in nonrelativistic quantum mechanics are divergent, yet asymptotic to  $E(\lambda)$  on some sector in the complex  $\lambda$  plane. Their large-order behavior is typically given by

$$E^{(n)} \sim (-1)^{n+1} A \Gamma(mn + \alpha) b^n, \quad n \rightarrow \infty, \quad (2.11)$$

where  $A, B, \alpha$ , and  $m$  are constants, with  $m = 1, 2, 3, \dots$ . Also,  $E(\lambda)$  is usually analytic in an appropriate sector of the complex  $\lambda$  plane, which includes the real  $\lambda$  line. This ensures the existence of the asymptotic expansion in Eq. (2.10) within the sector.<sup>23</sup> In many cases, the above properties can be used to establish the Borel summability<sup>24,25</sup> of perturbation series to  $E(\lambda)$  on some suitable sector of the complex  $\lambda$  plane which includes the positive real line.

Since we have been motivated in the past by the intimate relationship between continued fractions (CF) and RSPT,<sup>26</sup> this paper also considers the CF representations of the expansion given in Eqs. (2.7) and (2.8). These representations assume the form

$$E(\lambda) = E^{(0)} + \lambda C(\lambda), \quad (2.12)$$

where

$$C(z) = \frac{c_1}{1+} \frac{c_2 \lambda}{1+} \frac{c_3 \lambda}{1+} \dots \quad (2.13)$$

The reader is referred to Refs. 27 and 28 for comprehensive treatments of the analytic theory of continued fractions. The properties of continued fractions relevant to RSPT are given in Ref. 26.

The RS eigenvalue expansions for many standard perturbation problems, such as anharmonic oscillators, are negative Stieltjes for  $n \geq 1$ .<sup>7</sup> This implies that  $C(z)$  in Eq. (2.13) is an  $S$  fraction, i.e., all coefficients  $c_n$  are positive. Moreover, when the Stieltjes coefficients behave asymptotically as in Eq. (2.11), then<sup>26</sup>

$$c_n = O(n^m), \quad \text{as } n \rightarrow \infty. \quad (2.14)$$

In particular, when  $m = 1$ , then

$$c_n \sim \frac{1}{2} b n, \quad \text{as } n \rightarrow \infty. \quad (2.15)$$

When  $m < 2$ , Carleman's condition<sup>28</sup> is satisfied, which is sufficient to guarantee Padé summability of the RS series.

The convergents of  $C(z)$ , denoted  $w_n(z)$ , are obtained by truncating  $C(z)$ , i.e., setting  $c_{n+1} = 0$ . They are rational functions of  $z$ . The convergents  $w_{2N}(z)$  and  $w_{2N+1}(z)$  correspond, respectively, to the  $[N-1, N]$  and  $[N, N]$  Padé approximants<sup>29</sup> to the series being represented. If the series is a Stieltjes series,<sup>28</sup> then the sequences  $\{w_{2N}(z)\}$  and  $\{w_{2N+1}(z)\}$ ,  $N = 0, 1, 2, \dots$ , provide, respectively, lower and upper bounds to  $E(z)$ . If the series is Padé summable (corre-

sponding to determinacy of the moment problem), then these sequences converge to  $E(z)$  in the limit  $N \rightarrow \infty$ . The numerical calculations displayed in this report have used only continued fractions to "sum" the perturbation series.

### III. SPECIFIC APPLICATION TO NONLINEAR OSCILLATORS

In this section, we examine the perturbation expansions associated with the one-dimensional oscillators

$$\hat{H}^{(p,q)} = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + \lambda \langle x^{2p} \rangle x^{2q}, \quad (3.1)$$

with unperturbed energies  $E_K^{(0)} = K + \frac{1}{2}$ ,  $K = 0, 1, 2, \dots$ . The hypervirial relations in Eq. (2.6) become

$$\begin{aligned} (2k+1)E \langle x^{2k} \rangle &= (k+1) \langle x^{2k+2} \rangle + \lambda (q+2k+1) \langle x^{2(k+q)} \rangle \langle x^{2p} \rangle \\ &\quad - \frac{1}{4} k(2k+1)(2k-1) \langle x^{2k-2} \rangle, \\ k &= 0, 1, 2, \dots \end{aligned} \quad (3.2)$$

Since expectation values of odd powers of  $x$  vanish, we let

$$\langle x^{2k} \rangle = \sum_{n=0}^{\infty} C_k^{(n)} \lambda^n. \quad (3.3)$$

The HF theorem implies that

$$\frac{dE}{d\lambda} = \langle x^{2q} \rangle \frac{d}{d\lambda} [\lambda \langle x^{2p} \rangle]. \quad (3.4)$$

Equations (3.2)–(3.4) then yield the following recurrence relations for the  $C_k^{(n)}$  and the  $E^{(n)}$ :

$$\begin{aligned} k C_k^{(n)} &= (2k-1) \sum_{j=0}^n E^{(j)} C_{k-1}^{(n-j)} \\ &\quad - (q+2k-1) \sum_{j=0}^{n-1} C_p^{(j)} C_{q+k-1}^{(n-1-j)} \\ &\quad + \frac{1}{4} (k-1)(2k-1)(2k-3) C_{k-2}^{(n)}, \end{aligned} \quad (3.5)$$

$$E^{(n+1)} = \frac{1}{n+1} \sum_{j=0}^n (j+1) C_p^{(j)} C_q^{(n-j)}. \quad (3.6)$$

In order to determine  $E^{(n+1)}$ , one calculates the columns  $C_k^{(j)}$ , where  $j = 0, 1, \dots, n$ , and  $k = 1, 2, \dots, \max(p, q) + (n-j)q$ . Note that the entries  $C_k^{(0)}$  are the same for all perturbed oscillator problems, representing the unperturbed expectation values  $\langle x^{2k} \rangle(0)$  associated with the harmonic oscillator eigenfunctions. These expectation values are functions of the unperturbed eigenvalue  $E_K^{(0)}$ . The first five entries are given for reference in Table I. The  $C_i^{(j)}$  table and the RS coefficients  $E^{(n)}$  may be calculated in algebraic or in rational number form using a symbolic manipulation algorithm (the MAPLE language being developed at Waterloo<sup>30</sup> has been used for these purposes), or in floating-point form. Since the  $C_k^{(n)}$  will generally grow rapidly, especially as  $q$  in Eq. (3.1) increases, it may be necessary to avoid exponential overflow in floating-point calculations by scaling the coefficients. For example, define  $D_k^{(n)} = C_k^{(n)} s^{k+n}$ , where  $0 < s < 1$  is a scaling factor, conveniently some power of 10. Then rewrite the recursion relations (3.5) and (3.6) in

TABLE I. Expectation values  $\langle x^k \rangle$ ,  $k = 0, 1, \dots, 5$ , of the unperturbed harmonic oscillator eigenstates, expressed in terms of the unperturbed eigenvalue  $E_K^{(0)} = K + \frac{1}{2}$ . These entries define the first column of the  $C_K^{(n)}$  table in Eq. (3.5).

$k$	$C_K^{(0)} = \langle x^k \rangle (0)$
0	1
1	$t \equiv E_K^{(0)} = K + \frac{1}{2}$
2	$\frac{3}{2} t^2 + \frac{3}{8}$
3	$\frac{5}{8} t(4t^2 + 5)$
4	$\frac{35}{8} t^4 + \frac{245}{16} t^2 + \frac{315}{128}$
5	$\frac{63}{8} t^5 + \frac{945}{16} t^3 + \frac{2607}{128} t$

terms of the  $D_K^{(n)}$ . In this way, a set of scaled perturbation coefficients  $\bar{E}^{(n)} = s^n E^{(n)}$  is obtained.

### A. Nonlinear harmonic oscillators ( $q=1$ )

The Hamiltonians

$$\hat{H} = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + \lambda \langle x^{2p} \rangle x^2 \quad (3.7)$$

could be considered as describing harmonic oscillators with force constants directly proportional to mean values of powers of the vibrational amplitudes. Since the eigenvalues of the oscillators may be found exactly as roots of polynomials, they serve as a good testing ground for approximation methods. The special case  $p=q=1$  has been used by Cioslowski<sup>31</sup> to demonstrate a method of connected moments, and by Handy<sup>32</sup> for another method of moments.

The quantum mechanical virial theorem [ $k=0$  in Eq. (3.2)] states that for the harmonic oscillator (i.e.,  $\lambda=0$ ) in Eq. (3.7),  $\langle x^2 \rangle = E = E_K^{(0)}$ ,  $K=0,1,2,\dots$ . If the eigenvalue equation associated with (3.7) is scaled as  $x \rightarrow \alpha^{1/2} x$ ,  $\alpha \in \mathbb{R}$ , then

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} \alpha^2 (1 + 2\lambda \alpha^p \langle x^{2p} \rangle) x^2 \right] \psi = \alpha E \psi. \quad (3.8)$$

Choosing  $\alpha$  so that

$$\alpha^2 (1 + 2\lambda \alpha^p \langle x^{2p} \rangle) = 1, \quad (3.9)$$

we have  $\langle x^2 \rangle = \alpha E = E_K^{(0)}$ . (When  $\alpha=1$ , then  $E = E_K^{(0)}$ , our unperturbed state.) Equation (3.9) may be rewritten as  $E^{p+2} - (E_K^{(0)})^2 E^p - 2\lambda (E_K^{(0)})^{p+2} \langle x^{2p} \rangle = 0$ . (3.10)

Since the scaled Hamiltonian in (3.8) is a harmonic oscillator,  $\langle x^{2p} \rangle$  in (3.10) is a function of  $E_K^{(0)}$ . It has been given explicitly in Table I for  $p=0,1,\dots,5$ . The root of (3.10), which is a continuation of the unperturbed energy  $E_K^{(0)}$  for  $\lambda \neq 0$ , is the desired eigenvalue  $E(\lambda)$  of (3.7).

The RS expansions for  $E(\lambda)$  could be obtained either directly from the polynomial equations (3.10) or by the HVHF method. The radius of convergence of each expansion, to be denoted as  $R_p$  (possibly dependent upon the quantum number  $K$ ), will be the distance from  $\lambda=0$  to the nearest branch point singularities of (3.10), which will cor-

respond to the multiple roots. The  $R_p$  are easily determined in closed form for  $p=0,1,2$ . We summarize results below, presenting the first few terms of each RS expansion for  $E(\lambda)$ , its  $\lambda$  radius of convergence, and its continued fraction representation.

(i)  $p=0$ : The expansion is trivial here since  $E(\lambda) = (1 + 2\lambda)^{1/2} E_K^{(0)}$ ,  $R_p = \frac{1}{2}$ . We have

RSPT:  $E_K(\lambda)$

$$= E_K^{(0)} [1 + \lambda - \frac{1}{2} \lambda^2 + \frac{1}{2} \lambda^3 - \frac{5}{8} \lambda^4 + \frac{7}{8} \lambda^5 - \dots],$$

$$\text{CF: } E_K(\lambda) = E_K^{(0)} + \frac{E_K^{(0)} \lambda}{1 +} + \frac{\frac{1}{2} \lambda}{1 +} + \frac{\frac{1}{2} \lambda}{1 +} + \frac{\frac{1}{2} \lambda}{1 +} \dots$$

(ii)  $p=1$ : From (3.10),  $R_p = (3\sqrt{3} E_K^{(0)})^{-1}$ . We have

$$\text{RSPT: } E_K(\lambda) = E_K^{(0)} [1 + \beta - \frac{3}{2} \beta^2 + 4\beta^3 - \frac{195}{8} \beta^4 + 48\beta^5 - \dots],$$

$$\text{CF: } E_K(\lambda) = E_K^{(0)} + \frac{E_K^{(0)} \beta}{1 +} + \frac{\frac{3}{2} \beta}{1 +} + \frac{\frac{7}{6} \beta}{1 +} + \frac{\frac{59}{32} \beta}{1 +} + \frac{\frac{1005}{826} \beta}{1 +} \dots,$$

where  $\beta = \lambda E_K^{(0)}$ .

(iii)  $p=2$ :  $R_p = [8 \langle x^4 \rangle (0)]^{-1}$ . We have

$$\text{RSPT: } E_K(\lambda) = E_K^{(0)} [1 + g - \frac{5}{2} g^2 + \frac{21}{2} g^3 - \frac{429}{8} g^4 + \frac{2431}{8} g^5 - \dots],$$

$$\text{CF: } E_K(\lambda) = E_K^{(0)} + \frac{E_K^{(0)} g}{1 +} + \frac{\frac{5}{2} g}{1 +} + \frac{\frac{17}{10} g}{1 +} + \frac{\frac{381}{176} g}{1 +} + \frac{\frac{213525}{12954} g}{1 +} \dots,$$

where  $g = \lambda \langle x^4 \rangle (0) = \lambda [\frac{3}{2} (E_K^{(0)})^2 + \frac{3}{8}]$ .

In all cases, the continued fractions are  $S$  fractions. Numerical asymptotic analysis of the coefficients shows that  $c_n \rightarrow (4R_p)^{-1}$ . This behavior is consistent with Van Vleck's theorem (see Ref. 33, p. 138): Let  $C(z)$  be an  $S$  fraction such that  $\lim_{n \rightarrow \infty} c_n = a \neq 0$ ,  $a \in \mathbb{C}$ . Then the continued fraction  $C(z)$  converges to a function  $f(z)$  that is meromorphic (or identically infinite) in the cut complex plane  $C_a \equiv \{z: |\arg(az + \frac{1}{4})| < \pi\}$  (complex  $z$  plane with branch cut extending outward from  $z=a$  toward  $z=\infty$  on the line which is an extension of the line segment connecting  $z=a$  and  $z=0$  in the plane). The behavior of the  $c_n$  suggests that  $E(\lambda)$  is at least meromorphic in the complex  $\lambda$  plane with branch cut on  $(-\infty, -R_p)$ .

### B. Quartic anharmonic oscillators ( $q=2$ )

We now focus attention on the Hamiltonians

$$\hat{H}^{(p,2)} = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + \lambda \langle x^{2p} \rangle x^4, \quad p \geq 1, \quad (3.11)$$

and relate their eigenvalue expansions with those of the corresponding "linear" Bender-Wu (BW) oscillators<sup>4</sup> (with different normalization), where  $p=0$ :

$$\hat{H}^{(0,2)} = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + \lambda x^4. \quad (3.12)$$

The BW expansions associated with Eq. (3.12) will be denoted

$$E_K(\lambda) = \sum_{n=0}^{\infty} A_K^{(n)} \lambda^n, \quad (3.13)$$

$$\langle x^{2k} \rangle(\lambda) = \sum_{n=0}^{\infty} a_k^{(n)} \lambda^n. \quad (3.14)$$

The first three BW coefficients will be useful in this section:

$$\begin{aligned} A_K^{(0)} &= E_K^{(0)} = K + \frac{1}{2}, \quad A_K^{(1)} = \frac{3}{8} [4(E_K^{(0)})^2 + 1], \\ A_K^{(2)} &= -\frac{1}{16} E_K^{(0)} [68(E_K^{(0)})^2 + 67]. \end{aligned} \quad (3.15)$$

The large-order behavior of the  $A_K^{(n)}$  was first determined in Refs. 4 and 5 using WKB techniques [the RS series in Eq. (3.13) coincides with that of the original BW anharmonic oscillators]:

$$A_K^{(n)} \sim (-1)^{n+1} D_K \Gamma(n + K + \frac{1}{2}) 3^n [1 + O(1/n)], \quad (3.16)$$

where

$$D_K = (12^K / K!) (6/\pi^3)^{1/2}. \quad (3.17)$$

The series is Borel summable to  $E(\lambda)$  over the complex plane with cut on  $(-\infty, -B)$  for some  $B > 0$ .<sup>9</sup> The coefficients  $A_K^{(n)}$  are negative Stieltjes for  $n \geq 1$ , and the RS series is Padé summable to  $E(\lambda)$  on compact subsets of the cut plane  $|\arg \lambda| < \pi$ , the first Riemann sheet of  $E(\lambda)$ .<sup>8</sup> The continued fraction representation of the RS series is thus an  $S$  fraction, and its coefficients behave asymptotically as<sup>26</sup>

$$c_n \sim \frac{3}{2}n + \frac{3}{4}K + \frac{(-1)^n}{8}, \quad n \rightarrow \infty. \quad (3.18)$$

The hypervirial equations of (3.2) for the BW oscillator become

$$\begin{aligned} (2k+1)E \langle x^{2k} \rangle &= (k+1) \langle x^{2k+2} \rangle + \lambda(2k+3) \langle x^{2k+4} \rangle \\ &\quad - \frac{1}{4}k(2k+1)(2k-1) \langle x^{2k-2} \rangle, \\ k &= 0, 1, 2, \dots \end{aligned} \quad (3.19)$$

From the Hellmann–Feynmann theorem,  $dE/d\lambda = \langle x^4 \rangle$ , we have the result

$$a_2^{(n)} \sim (-1)^n D_K \Gamma(n + K + \frac{5}{2}) 3^{n+1}, \quad n \rightarrow \infty. \quad (3.20)$$

By setting  $k=0$  in Eq. (3.19) we also find that

$$a_1^{(n)} \sim (-1)^n D_K \Gamma(n + K + \frac{3}{2}) 3^{n+1}, \quad n \rightarrow \infty. \quad (3.21)$$

From these results, and from a repeated application of the difference equation for the  $C_p^{(j)}$  associated with Eq. (3.19), we arrive at the following general result for the large-order behavior of the expansion coefficients in (3.14):

$$a_k^{(n)} \sim (-1)^n B_k D_K \Gamma(n + K + \frac{1}{2} + k) 3^{n+1}, \quad n \rightarrow \infty, \quad (3.22)$$

where  $B_1 = B_2 = 1$ , and

$$B_k = \prod_{j=3}^k \frac{(j-1)}{(2j-1)}, \quad k \geq 3. \quad (3.23)$$

This formula has also been verified by numerical asymptotic analysis of the  $a_k^{(n)}$ , for  $k = 1, 2, \dots, 5$ . The analyticity of  $E(\lambda)$  along with the recursion relation (3.19) ensures analyticity of  $\langle x^{2k} \rangle(\lambda)$ ,  $k = 1, 2, 3, \dots$ , on the cut plane,  $|\arg \lambda| < \pi$ . The large-order behavior of the  $a_k^{(n)}$  in (3.22) establishes Borel summability of the expansions in (3.14) to  $\langle x^{2k} \rangle(\lambda)$  on a strip which contains the real  $\lambda$  line.

The continued fraction representations of the  $\langle x^{2k} \rangle$  series, having the form

$$\langle x^{2k} \rangle(\lambda) = C_k(\lambda) = \frac{c_{k1}}{1 +} \frac{c_{k2}\lambda}{1 +} \frac{c_{k3}\lambda}{1 +} \dots, \quad (3.24)$$

have also been computed to order  $n = 70$  for  $k = 1, 2, \dots, 5$ . In all cases, the  $C_k(\lambda)$  are observed to be  $S$  fractions. Numerical asymptotic analysis indicates that

$$c_{kn} \sim \frac{3}{2}n + O(1), \quad n \rightarrow \infty. \quad (3.25)$$

On the basis of this numerical evidence, we conjecture the Stieltjes nature of the  $\langle x^{2k} \rangle$  expansions in (3.14). The  $n!$  growth of the coefficients  $a_k^{(n)}$  for  $k \geq 1$  suggests the Padé summability of the series over compact subsets of the cut plane  $|\arg \lambda| < \pi$ , in accordance with Carleman's condition.<sup>28</sup>

The properties of the BW oscillator expansions will now be useful for an understanding of the nonlinear problems in Eq. (3.11). For notational convenience, indices referring to  $p$  and  $q$  as well as to the quantum number  $K$  will be omitted unless there may be an ambiguity. The nonlinear problems may be considered to define a new coupling constant  $\beta$ ,

$$\beta = \lambda \langle x^{2p} \rangle = \sum_{n=0}^{\infty} C_p^{(n)} \lambda^{n+1}. \quad (3.26)$$

To lowest order in  $\lambda$ ,  $\beta \sim C_p^{(0)} \lambda$ , so that we would expect the geometric factor  $3^k$  in Eqs. (3.15) and (3.22) to be replaced by  $(3C_p^{(0)})^k$ . This will indeed be verified below. A formal relationship between the “nonlinear” RS coefficients  $E^{(n)}$  and the BW coefficients  $A^{(n)}$  may be obtained by equating powers of  $\lambda^n$  in the relation

$$E(\lambda) = \sum_{n=0}^{\infty} E^{(n)} \lambda^n = \sum_{j=0}^{\infty} A^{(j)} \beta^j. \quad (3.27)$$

If we set  $g_n \equiv C_p^{(n)}$ , then the first few relations become

$$\begin{aligned} E^{(0)} &= A^{(0)}, \quad E^{(1)} = A^{(1)} g_0, \\ E^{(2)} &= A^{(1)} g_1 + A^{(2)} g_0^2, \\ E^{(3)} &= A^{(1)} g_2 + 2A^{(2)} g_0 g_1 + A^{(3)} g_0^3. \end{aligned} \quad (3.28)$$

The general formula for  $E^{(n)}$ ,  $n \geq 1$ , in (3.28) may be written as

$$\begin{aligned} \frac{E^{(n)}}{A^{(n)} g_0^{(n)}} &= \left[ \sum_{k=0}^n \binom{n-1}{k} \frac{A^{(n-k)}}{A^{(n)}} \left( \frac{g_1}{g_0^2} \right)^k \right] \\ &\quad + \frac{A^{(1)}}{A^{(n)}} \frac{g_{n-1}}{g_0^n} + \frac{2A^{(2)}}{A^{(n)}} \frac{g_{n-2}}{g_0^{n-1}} + \dots \end{aligned} \quad (3.29)$$

The pattern exhibited in these equations indicates that the asymptotic behavior of the  $E^{(n)}$  will be dependent upon  $g_n = C_p^{(n)}$  as well as the  $A^{(n)}$ . From Eq. (3.16), the partial sum in square brackets becomes, in the limit  $n \rightarrow \infty$ ,  $\exp(-g_1/(3g_0^2))$ . It now remains to determine the asymptotics implied by the remaining terms, which will be done below for the particular cases  $p = 1, 2$ . Keeping in mind the behavior of the “linear” expectation series coefficients  $a_k^{(n)}$  in Eq. (3.22) and the remarks following Eq. (3.26), two assumptions on the asymptotic behavior of the  $g_n$  will be made in the analysis to follow:

$$C_{p+1}^{(n)}/C_p^{(n)} \sim O(n), \quad \text{as } n \rightarrow \infty, \quad (3.30a)$$

$$\lim_{n \rightarrow \infty} (g_{n+1}/ng_n) = -3g_0, \quad (3.30b)$$

the latter implying an  $n!$  growth of the form (3.26), replacing the geometric term 3 by  $3g_0$ .

Case 1:  $p = 1, g_n \equiv C_1^{(n)}$ . First, rewrite (3.30) as

$$\frac{E^{(n)}}{A^{(n)}g_0^n} \left[ 1 - A^{(1)} \frac{g_{n-1}}{E^{(n)}} \right] \sim e^{-g_1/(3g_0^2)}, \quad (3.31)$$

where we have used (3.29) to ignore the contributions of the remaining terms in (3.30). The relevant parameters are  $g_0 = E^{(0)}$  and  $g_1 = -2E^{(0)}A^{(1)}$ . It now remains to determine the asymptotic behavior of the second term in square brackets. From the hypervirial relation [ $k = 0$  in Eq. (3.2)]

$$E = \langle x^2 \rangle + 3\lambda \langle x^2 \rangle \langle x^4 \rangle, \quad (3.32)$$

it follows that

$$\begin{aligned} \frac{E^{(n)}}{C_1^{(n-1)}} &= \frac{C_1^{(n)}}{C_1^{(n-1)}} + 3C_1^{(1)} \frac{C_2^{(n-1)}}{C_1^{(n-1)}} \\ &+ 3 \frac{C_2^{(n-2)}}{C_1^{(n-1)}} + 3C_2^{(0)} + O\left(\frac{1}{n}\right). \end{aligned} \quad (3.33)$$

From Eq. (3.6) we also have

$$\frac{E^{(n)}}{C_1^{(n-1)}} = \frac{C_1^{(0)}C_2^{(n-1)}}{nC_1^{(n-1)}} + C_2^{(0)} + O\left(\frac{1}{n}\right). \quad (3.34)$$

From the two assumptions in Eq. (3.30), the first two terms on the rhs of (3.33) behave as  $O(n)$ . Equating (3.33) and (3.34), and using (3.29), reveals that

$$C_2^{(n-1)}/nC_1^{(n-1)} \sim 1, \quad \text{as } n \rightarrow \infty. \quad (3.35)$$

From Eq. (3.34), and the fact that  $C_2^{(0)} = A^{(1)}$ ,

$$E^{(n)}/C_1^{(n-1)} = A^{(0)} + A^{(1)}, \quad (3.36)$$

which, when substituted into (3.31), gives

$$\begin{aligned} E_K^{(n)} &\sim [1 + A_K^{(1)}/A_K^{(0)}] \\ &\times \exp[2A_K^{(1)}/3A_K^{(0)}] (A_K^{(0)})^n A_K^{(n)}, \quad \text{as } n \rightarrow \infty. \end{aligned} \quad (3.37)$$

This formula has been verified by numerical asymptotic analysis of the expansions corresponding to  $K = 0, 1, \dots, 6$ .

Case 2:  $p = 2, g_n \equiv C_2^{(n)}$ . From Eq. (3.6), we have

$$E^{(n)} = \frac{1}{n} \sum_{j=0}^{n-1} (j+1)g_j g_{n-1-j}, \quad (3.38)$$

so that

$$\frac{E^{(n)}}{g_{n-1}} = g_0 + \left[ g_0 - \frac{g_1}{3g_0} \right] \frac{1}{n} + O\left(\frac{1}{n}\right). \quad (3.39)$$

Also,

$$\frac{E^{(n)}}{g_{n-2}} = \frac{E^{(n)}}{g_{n-1}} \frac{g_{n-1}}{g_{n-2}} = \frac{E^{(n)}}{g_{n-1}} [-3ng_0 + O(1)]. \quad (3.40)$$

Equation (3.29) is then rewritten as

$$\frac{E^{(n)}}{A^{(n)}g_0^n} \left[ 1 - A^{(1)} \frac{g_{n-1}}{E^{(n)}} - 2A^{(2)}g_0 \frac{g_{n-2}}{E^{(n)}} \right] \sim e^{-g_1/(3g_0^2)}, \quad n \rightarrow \infty. \quad (3.41)$$

[Note the difference between (3.41) and (3.31).] For this case we compute  $g_0 = A^{(1)}$  and  $g_1 = 2A^{(2)}A^{(1)}$ , so that the term in square brackets reduces to  $A^{(1)}/(g_0n) = 1/n$ . The net result is

$$E_K^{(n)} \sim n \exp[-2A_K^{(2)}/3A_K^{(1)}] (A_K^{(1)})^n A_K^{(n)}, \quad n \rightarrow \infty, \quad (3.42)$$

which we may write as

$$\begin{aligned} E_K^{(n)} &\sim (-1)^{n+1} \exp[-2A_K^{(2)}/3A_K^{(1)}] \\ &\times D_K \Gamma(n + K + \frac{3}{2}) (3A_K^{(1)})^n, \quad n \rightarrow \infty. \end{aligned} \quad (3.43)$$

A final note must be made concerning the relations in (3.37) and (3.43). The exponential factors occurring in these relations can easily be obtained by substituting the relevant form of Eq. (3.26) into the Bender–Wu formula for the asymptotics of  $\text{Im } E(\lambda)$ ,  $\lambda \rightarrow 0^-$  [cf. Eq. (A8), p. 1635 of Ref. 4(b)]. However, this naive treatment ignores the contribution of terms such as  $g_{n-1}$  in Eq. (3.29) or (3.31).

#### IV. APPLICATIONS TO RADIAL HYDROGENIC PROBLEMS

The application of the HVHF and renormalization methods to the ( $N$ -dimensional) hydrogenic problems

$$\hat{H}^{(p,q)} = \frac{1}{2} \hat{p}_r^2 + \frac{\hat{L}^2}{2r^2} - \frac{Z}{r} + \lambda \langle r^p \rangle r^q \quad (4.1)$$

is quite straightforward. Our treatment will be restricted to three-dimensional problems. The cases  $p = 0$  correspond to generalized charmonium problems.<sup>34</sup> After a factorization of angular terms, the hypervirial relations of Eq. (2.6) become

$$\begin{aligned} 2(k+1)E \langle r^k \rangle &= -(2k+1)Z \langle r^{k-1} \rangle + (2k+q+2)\lambda \langle r^p \rangle \langle r^{k+q} \rangle \\ &+ k[L(L+1) - \frac{1}{4}(k+1)(k-1)] \langle r^{k-2} \rangle, \\ k &\in \mathbb{Z}, \end{aligned} \quad (4.2)$$

where  $E = E_{NLM}(\lambda)$  represents the eigenvalue arising from the perturbation of the bound state hydrogenic eigenfunction  $\psi_{NLM}^{(0)}$  with eigenvalue  $E_{NLM}^{(0)} = -Z^2/(2N^2)$  [ $N, L$ , and  $M$  will denote the usual hydrogenic quantum numbers, so  $L(L+1)$  replaces the scalar  $L^2$  in Eq. (2.3)]. When the expansions

$$\langle r^k \rangle = \sum_{n=0}^{\infty} C_k^{(n)} \lambda^n \quad (4.3)$$

are assumed, the difference equations for the  $C_k^{(n)}$  and  $E^{(n)}$  become

$$\begin{aligned} 2(k+1)E^{(0)}C_k^{(n)} &= -2(k+1) \sum_{j=1}^n E^{(j)} C_k^{(n-j)} - (2k+1)Z C_{k-1}^{(n)} \\ &+ (2k+1+2) \sum_{j=1}^{n-1} C_p^{(j)} C_{q+k}^{(n-1-j)} \\ &+ k[L(L+1) - \frac{1}{4}(k+1)(k-1)] C_{k-2}^{(n)}, \end{aligned} \quad (4.4)$$

$$E^{(n+1)} = \frac{1}{n+1} \sum_{j=0}^n (j+1) C_p^{(j)} C_q^{(n-j)}. \quad (4.5)$$

The calculation of the  $C_k^{(n)}$  array proceeds columnwise as for the oscillator problems, with the exception that the row corresponding to  $k = -1$  must now be included. At the beginning of each order of calculation  $n$ , we use the formula [ $k = 0$  in (4.2)]

$$c_{-1}^{(n)} = \frac{1}{Z} \left[ -2E^{(n)} + (q+2) \sum_{j=0}^{n-1} c_p^{(j)} c_q^{(n-1-j)} \right].$$

We shall consider in particular the Hamiltonians ( $Z = 1$ )

$$\hat{H} = \frac{1}{2} \hat{p}_r^2 + \frac{\hat{L}^2}{2r^2} - \frac{1}{r} + \lambda \langle r^p \rangle r, \quad p = 0, 1, 2, \quad (4.6)$$

and relate their perturbation expansions with those of the "charmonium" problem,<sup>34</sup>

$$\hat{H} = \frac{1}{2} \hat{p}_r^2 + \frac{\hat{L}^2}{2r^2} - \frac{1}{r} + \lambda r. \quad (4.7)$$

The expansions associated with the "linear" eigenvalue problem (4.7) will be denoted as

$$E_{NLM}(\lambda) = \sum_{n=0}^{\infty} A_{NLM}^{(n)} \lambda^n, \quad (4.8)$$

$$\langle r^k \rangle(\lambda) = \sum_{n=0}^{\infty} a_k^{(n)} \lambda^n, \quad k \geq -1. \quad (4.9)$$

The first three coefficients of the eigenvalue expansion are given by

$$\begin{aligned} A_{NLM}^{(0)} &= -1/2N^2, \\ A_{NLM}^{(1)} &= \frac{3}{2}N^2 - \frac{1}{2}L(L+1), \\ A_{NLM}^{(2)} &= -\frac{7}{8}N^6 + \frac{3}{8}[L(L+1)]^2N^2 - \frac{5}{8}N^4. \end{aligned} \quad (4.10)$$

The large-order behavior of the  $A_{NLM}^{(n)}$  is given by<sup>35</sup>

$$A_{NLM}^{(n)} \sim (-1)^{n+1} D_{NLM} \Gamma(n+2N) (\frac{3}{2}N^3)^n, \quad n \rightarrow \infty, \quad (4.11)$$

where

$$D_{NLM} = \frac{3^{2N} 2^{2N-1} e^{-3N+L(L+1)/N}}{\pi N^3 (N+L)! (N-L-1)!}. \quad (4.12)$$

The RS coefficients are negative Stieltjes for  $n \geq 1$ , and the series is Padé summable to  $E(\lambda)$  on the cut plane  $|\arg \lambda| < \pi$ . The coefficients of the  $S$  fraction representation to  $E(\lambda)$  behave asymptotically as

$$c_n \sim \frac{3}{4}N^3 n + K^{(i)}, \quad i = \begin{cases} 1, & n \text{ even}, \\ 2, & n \text{ odd}, \end{cases} \quad (4.13)$$

where

$$K^{(1)} = \frac{3}{2}N^4 - \frac{1}{2}N^3, \quad K^{(2)} = \frac{3}{2}N^4 - \frac{1}{4}N^3.$$

We now determine the asymptotic behavior of the expansion coefficients  $a_k^{(n)}$  in Eq. (4.9), in a manner similar to that used for the oscillator problems. The hypervirial equations to be used for the linear charmonium problem are

$$\begin{aligned} 2(k+1)E \langle r^k \rangle &= -(2k+1) \langle r^{k-1} \rangle + (2k+3) \lambda \langle r^{k+1} \rangle \\ &\quad + k [L(L+1) - \frac{1}{4}(k+1)(k-1)] \langle r^{k-2} \rangle, \\ k &\geq -1. \end{aligned} \quad (4.14)$$

From the Hellmann-Feynman theorem,  $dE/d\lambda = \langle r \rangle$ , it follows that

$$a_1^{(n)} \sim (-1)^n D_{NLM} \Gamma(n+N+2) (\frac{3}{2}N^3)^{n+1}, \quad n \rightarrow \infty. \quad (4.15)$$

This implies that, for  $k \geq 1$ ,

$$a_{k+1}^{(n-1)}/a_k^{(n)} \sim [2(k+1)/(2k+3)] E^{(0)}, \quad n \rightarrow \infty. \quad (4.16)$$

Repeated application of this property leads to the following asymptotic formulas:

$$a_k^{(n)} \sim (-1)^n B_k D_{NLM} \Gamma(n+N+k+1) (\frac{3}{2}N^3)^{n+1}, \quad (4.17)$$

where  $B_1 = 1$  and

$$B_k = \left( \frac{3}{4} N \right)^{k-1} \prod_{j=1}^k \frac{2(j+1)}{2j+3}, \quad k \geq 2. \quad (4.18)$$

This formula has been verified by numerical asymptotic analysis of the  $a_k^{(n)}$  for  $k = 1, 2, \dots, 5$ .

Analyticity of the functions  $\langle r^k \rangle(\lambda)$ ,  $k \geq 1$ , in the cut plane  $|\arg \lambda| < \pi$  follows from the analyticity properties of  $E(\lambda)$  and the recursion relation in (4.14). We also conjecture that their series expansions in (4.9) are Stieltjes. This is based on the numerical evidence that the continued fraction representations of  $\langle r^k \rangle$  having the same form as in Eq. (3.24) are  $S$  fractions. The coefficients  $c_{kn}$  have been computed accurately to order  $n = 70$  for  $k = 1, 2, \dots, 5$ . In all cases, the generic asymptotic growth of Eq. (4.13) is observed. The  $n!$  growth of the  $a_k^{(n)}$  satisfies Carleman's condition which would imply Padé summability on compact subsets of the cut plane  $|\arg \lambda| < \pi$ . Convergence of  $[N-1, N]$  and  $[N, N]$  Padé approximants to  $\langle r^k \rangle$  for  $k = -1, 1, 2$  were first observed by Austin.<sup>14</sup>

The behavior of the series expansion for  $\langle r^{-1} \rangle$  stands apart from those described above. By setting  $k = 0$  in Eq. (4.14) and comparing Eqs. (4.11) and (4.15), it follows that  $a_{-1}^{(n)} \sim 3nE^{(n)}$ , or

$$a_{-1}^{(n)} \sim (-1)^{n+1} 3D_{NLM} \Gamma(n+N+1) (\frac{3}{2}N^3)^n, \quad n \rightarrow \infty. \quad (4.19)$$

Since  $a_{-1}^{(1)}$  is positive, we consider CF representations of the form

$$\langle r^{-1} \rangle(\lambda) = 1/N^2 + C_{-1}(\lambda), \quad (4.20)$$

where  $C(\lambda)$  has the usual form in Eq. (2.13). All CF representations are observed to be  $S$  fractions. Their coefficients behave asymptotically as in Eq. (4.13), in accordance with the large-order behavior in Eq. (4.19).

The analysis of perturbation expansions for the nonlinear problems in (4.1) now proceeds as in Sec. III B. The nonlinear problems define the new coupling constant  $\beta$ ,

$$\beta = \lambda \langle r^p \rangle = \sum_{n=0}^{\infty} C_p^{(n)} \lambda^{n+1} \equiv \sum_{n=0}^{\infty} g_n \lambda^{n+1}. \quad (4.21)$$

The formal relations of Eqs. (3.27) and (3.28) apply, and the assumptions similar to Eq. (3.30) of the oscillator problems are made, with the following minor modification:

$$\lim_{n \rightarrow \infty} (g_{n+1}/ng_n) = -cg_0, \quad (4.22)$$

where  $c = \frac{3}{2}N^3$ .



We shall now employ Eq. (3.29) and elucidate the asymptotics for the particular case  $p = 1$ . The relevant parameters are  $g_0 = A^{(1)}$  and  $g_1 = 2A^{(1)}A^{(2)}$ . This case is seen to be analogous to case 2 of Sec. III B. The net result is [cf. Eq. (3.42)]

$$E^{(n)} \sim \exp[-g_1/3g_0^2] n A^{(n)} g_0^n, \quad n \rightarrow \infty. \quad (4.23)$$

This may be written as

$$E_{NLM}^{(n)} \sim (-1)^{n+1} D_{NLM} \exp[-\frac{2}{3} A_{NLM}^{(2)}/A_{NLM}^{(1)}] \times \Gamma(n+2N+1) [\frac{2}{3} N^3 A_{NLM}^{(1)}]^n, \quad n \rightarrow \infty. \quad (4.24)$$

## V. RENORMALIZED RSPT AND EIGENVALUES OF INFINITE FIELD HAMILTONIANS

An examination of the region of analyticity of eigenvalues  $E(\lambda)$  and the nature of their RS perturbation expansions can establish the theoretical summability of these expansions. From a practical aspect, however, RSPT, being a “low-field” expansion, can be relied upon to furnish accurate estimates of  $E(\lambda)$  only for small values of the coupling constant  $\lambda$ . Methods for accelerating the convergence of these summability methods may increase this region of  $\lambda$  values by perhaps an order of magnitude. Recently,<sup>36</sup> a “renormalized” perturbation theory has been devised to permit accurate perturbative calculations of  $E(\lambda)$  over an infinite range of  $\lambda$  values. It has been applied successfully to the “linear” oscillator and hydrogenic problems and will now be applied to the nonlinear oscillator problems introduced above. The goal is to calculate (1) the eigenvalues  $E_K^{(p,q)}(\lambda)$  of the Hamiltonians in Eq. (3.1) accurately over the entire real interval  $0 \leq \lambda < \infty$ , and (2) the eigenvalues  $F_K^{(p,q)(0)}$  of the “infinite-field” Hamiltonians corresponding to the nonlinear oscillators of above, i.e.,

$$\hat{H}_\infty^{(p,q)} = -\frac{1}{2} \frac{d^2}{dx^2} + \langle x^{2p} \rangle x^{2q}. \quad (5.1)$$

The technical discussions of this method of renormalization, presented in Ref. 30, are omitted. Again it is emphasized that only continued fractions were employed for the following numerical calculations. Padé summability is expected to break down for  $q > 2$ , however. An examination of other summability methods, including Borel, is currently in progress.

The eigenvalues  $F_K^{(p,q)(0)}$  of (5.1) are significant for the following reason. A scaling  $x \rightarrow \alpha^{1/2} x$ , where  $\alpha = \lambda^{-1/(p+q+1)}$ ,  $\lambda > 0$  (representing a unitary transformation), may be applied to the eigenvalue problems associated with (3.1) to give

$$E_K^{(p,q)}(\lambda) \sim F_K^{(p,q)} \lambda^{1/(p+q+1)}, \quad \text{as } \lambda \rightarrow \infty. \quad (5.2)$$

[Under this coordinate transformation,  $\langle x^{2p} \rangle$  scales as  $\alpha^p$ , by its definition in Eq. (1.5).] This is, in fact, but the leading term in the infinite-field expansion

$$E_K^{(p,q)}(\lambda) = \lambda^{1/(p+q+1)} \sum_{k=0}^{\infty} F_K^{(p,q)(k)} \lambda^{-2k/(p+q+1)}, \quad (5.3)$$

which, for  $q \geq 2$ , should be convergent for  $|\lambda| > R > 0$ .<sup>7</sup>

We now outline a method to calculate the  $F_K^{(p,q)(0)}$ . First, construct the “renormalized” Schrödinger equation [dropping the  $(p,q)$  and  $K$  indices for notational convenience]:

$$\begin{aligned} \hat{H}_R(\beta) \psi \\ = \left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + \beta \left( \langle x^{2p} \rangle x^{2q} - \frac{1}{2} x^2 \right) \right] \psi \\ = G(\beta), \end{aligned} \quad (5.4)$$

so that the  $G^{(p,q)}(1)$  correspond to the eigenvalues of  $H_\infty^{(p,q)}$  in (5.1). Now assume an RS perturbation expansion of the form

$$G(\beta) = \sum_{n=0}^{\infty} G^{(n)} \lambda^n \quad (5.5)$$

for each eigenstate. By scaling the coordinates in (5.4) as  $x \rightarrow \tau^{1/2} x$ , where  $0 \leq \tau^2 = 1 - \beta < 1$ , the eigenvalues of (5.4) and (3.1) are related as

$$G_K(\beta) = (1 - \beta)^{1/2} E(\beta / (1 - \beta)^{(p+q+1)/2}). \quad (5.6)$$

This relation effectively defines a renormalization map  $R: \beta \rightarrow \lambda$  which, restricted to the nonnegative real line, maps  $\beta \in [0, 1]$  onto  $\lambda \in [0, \infty)$ . By equating the series in (1.6) and (5.5) termwise, and using the general binomial expansion

$$(1 - \beta)^{-\alpha} = \sum_{k=0}^{\infty} \frac{\Gamma(\alpha + k)}{\Gamma(\alpha) \Gamma(k + 1)} \beta^k, \quad (5.7)$$

we find the relation

$$G^{(n)} = \sum_{k=0}^n \frac{\Gamma(k(p+q-1)/2 + n - \frac{1}{2})}{\Gamma(k(p+q+1)/2 - \frac{1}{2}) \Gamma(n-k-1)} E^{(n)}. \quad (5.8)$$

A similar type of renormalization and linear transformation (5.8) occurs in the case of Wick-ordered perturbation series associated with simple field theories.<sup>7,37</sup> The renormalized series coefficients  $G^{(n)}$  could, in principle, be calculated from the  $E^{(k)}$  by the above relation. Practically speaking, however, the HVHF method is easily applied to the perturbation problem in Eq. (5.4), requiring but a minor modification of the difference equations (3.5) and (3.6). An asymptotic analysis of Eq. (5.8) reveals that  $G^{(n)} = O(E^{(n)})$  as  $n \rightarrow \infty$ .

Again, we have not rigorously established the summability of the RS  $\lambda$  series or the renormalized  $\beta$  series for the nonlinear oscillator problems. In Ref. 36, it is shown, using a theorem of Sokal,<sup>38</sup> that if the  $\lambda$  series is Borel summable, then the  $\beta$  series is Borel summable in  $[0, 1]$ .

In Table II are presented estimates of the eigenvalues  $F_K^{(p,q)(0)}$  of the Hamiltonians  $H_\infty^{(p,q)}$  in Eq. (5.1) for  $p = 0, 1, 2$ ,  $q = 2$  (quartic anharmonic oscillators). These estimates were obtained from the convergents  $w_{49}(1)$  and  $w_{50}(1)$  to the continued fraction representation of the renormalized  $\beta$  series in Eq. (5.5). A slight “trick” was employed here, as described in Ref. 36, so that the continued fractions were  $S$  fractions: for oscillator problems such as (4.4), the perturbation  $W(x) = \langle x^{2p} \rangle x^{2q} - \frac{1}{2} x^2$  is not positive definite, since  $W(x) < 0$  for  $x \ll 1$ . To overcome this difficulty,

TABLE II. Lower and upper bounds to the eigenvalues  $F_K^{(p,2)(0)}$  of the infinite field Hamiltonian  $\hat{H}^{(p,2)}$  as defined in Eq. (5.1). The lower and upper bounds are obtained from the convergents  $w_{50}(1)$  and  $w_{49}(1)$ , respectively, of the continued fraction representation of the renormalized  $\beta$  series in Eq. (5.5). The actual numerical entries are the lower bounds. Replacing the final  $n$  digits of the entry by the  $n$  digits in parentheses gives the upper bound. The entries in parentheses below the  $p = 0$  row are numerical values calculated by Bell *et al.*<sup>39</sup> and Reid<sup>40</sup> (scaled appropriately due to a different normalization). The estimate  $0.489\,05 < F_K^{(1,2)(0)} < 0.489\,07$  has been obtained by Handy<sup>32</sup> using a method of moments.

$p$	$K$		
	0	1	2
0	0.667 95(801) (0.667 986)	2.393 47(84) (2.393 644)	4.696 1(76) (4.696 795)
1	0.489 0640(36)	2.200 9(28)	4.67(71)
2	0.494 64(5)	2.27(31)	4.9(5.7)
3	0.534 4(59)	2.35(79)	

we “shift” the perturbation up by an amount  $\Delta = \beta g$ ,  $g > 0$ , to guarantee that  $W(x) > 0$  for all  $x \neq 0$ . We thus consider the modified series expansion

$$G(\beta) = G^{(0)} = \beta g + \sum_{n=1}^{\infty} \bar{G}^{(n)} \beta^n, \quad (5.9)$$

where  $\bar{G}^{(1)} = G^{(1)} + g$ ,  $\bar{G}^{(k)} = G^{(k)}$  for  $k \geq 2$ . Typically, we have chosen  $g = E^{(0)}$ . This choice is somewhat arbitrary, but it ensures that the minimum of  $W(x)$  is nonnegative. For the “linear” problems, where  $p = 0$ , we can calculate the minimum value of  $g$  that guarantees positivity of  $W(x)$ .<sup>36</sup> In all cases, the CF representation is found to be an  $S$  fraction. The upper and lower bounds yielded by the convergents  $w_{49}(1)$  and  $w_{50}(1)$ , respectively, are given in Table II. The eigenvalues  $F_K^{(0,2)}$  have been calculated accurately by Bell *et al.*<sup>39</sup> and Reid.<sup>40</sup> These values are included in Table II for reference. (Because of a different scaling of the Hamiltonian, the eigenvalues reported in these papers must be divided by the factor  $2^{2/3}$ .) Recently, Handy<sup>32</sup> has independently obtained the ap-

proximate value  $0.490\,45 < F_0^{(1,2)} < 0.490\,47$  using a method of moments.

The renormalization relation in (5.6) may also be employed to calculate the eigenvalues  $E_K^{(p,q)}(\lambda)$  over the entire range  $0 < \lambda < \infty$ . We “invert” the scaling transformation  $x \rightarrow \tau^{1/2}x$ ,  $\tau^2 = 1 - \beta$ , used to derive Eq. (5.6), to obtain

$$E(\lambda) = \tau^{-1}G(1 - \tau^2), \quad (5.10)$$

where  $\tau$  is the root of the equation

$$\lambda \tau^{p+q+1} + \tau^2 - 1 = 0, \quad (5.11)$$

which satisfies  $\tau = 1$  when  $\lambda = 0$ ,  $\tau \rightarrow 0$  as  $\lambda \rightarrow \infty$ . In fact,  $\tau \sim \lambda^{-1/(p+q+1)}$  as  $\lambda \rightarrow \infty$ . In order to calculate  $E_K^{(p,q)}(\lambda)$ , we then (i) calculate the renormalized coefficients  $G_K^{(p,q)(k)}$  by HVHF applied to Eq. (5.4); (ii) compute  $\tau$  from Eq. (5.11) to a prescribed accuracy using the Newton–Raphson method; (iii) “sum” the  $\beta$  series by using Borel, Padé, or other summability techniques; and (iv) compute  $E(\lambda)$  from (5.10).

In Table III are presented the estimates of  $E_0^{(p,q)}(\lambda)$  for  $q = 2$ ,  $p = 0, 1$ , a range of  $\lambda$  values. The maximum error in these calculations is expected to be incurred in the high-field limit, i.e.,  $\beta = 1$ . Thus, for a given value of  $p$ , the errors in the estimates of  $E(\lambda)$  for  $0 < \infty$  will be less than for those given in Table II. For  $\lambda = 10\,000$ , the values  $\lambda^{-1/(p+2+1)}E_K^{(p,2)}(\lambda)$  approximate the eigenvalues  $F_K^{(p,2)(0)}$  of Table II quite well. The relative behavior of the ground state eigenvalues  $E_0^{(p,q)}(\lambda)$  for  $0 \leq \lambda \leq 3$ ,  $p = 0, \dots, 4$ , is shown in Fig. 1.

## VI. CONCLUDING REMARKS

The model Hamiltonians studied here are very simplified versions of those used to model self-interacting systems. The large-order behavior of Rayleigh–Schrödinger eigenvalue expansions may be related to that of the associated linear eigenvalue problems. This is expected since the nonlinearity of these problems is quite “tame,” manifesting itself as a modified coupling constant. The analysis was performed

TABLE III. Estimates of ground-state eigenvalues  $E_0^{(p,2)}(\lambda)$  of one-dimensional quartic anharmonic oscillators in Eq. (3.11) for  $p = 0$  (“linear” Bender–Wu case), 1, 2, and 3. The entries represent the lower bound estimates afforded by the [24,25] ( $\beta$ ) Padé approximant to the renormalized  $\beta$  series in Eq. (4.5), with  $\beta = 1 - \tau^2$  and  $\tau$  being the root of Eq. (4.10). Replacing the final  $n$  digits in each entry with the  $n$  digits in the accompanying parentheses gives the upper bound estimate yielded by the [24,24] ( $\beta$ ) Padé.

$\lambda$	0	1	2	3
0.1	0.559 146 327 183519(21)	0.529 717 430 561 641	0.536 324 651 544 448(9)	0.556 718 751 80(6)
0.5	0.696 175 816(25)	0.597 374 410 315(6)	0.600 619 895 9(61)	0.627 289 6(905)
1.0	0.803 770 5(7)	0.649 058 485 4(5)	0.644 396 19(20)	0.670 209(17)
2.0	0.951 567(9)	0.718 266 089(90)	0.699 718 64(72)	0.721 69(73)
3.0	1.060 263(9)	0.768 002 287(92)	0.737 969 56(74)	0.756 09(16)
4.0	1.148 78(9)	0.807 851 82(3)	0.767 944 7(51)	0.782 5(6)
5.0	1.224 578(94)	0.841 539 59(61)	0.792 897 0(5)	0.804 2(4)
10.0	1.504 95(9)	0.963 031 00(6)	0.880 525(7)	0.878 8(91)
20.0	1.865 65(73)	1.113 125 1(3)	0.984 887(91)	0.964 9(55)
50.0	2.499 6(8)	1.363 503 3(6)	1.152 113(20)	1.099 5(95)
100.0	3.131 26(47)	1.599 659 0(6)	1.303 94(5)	1.216 4(78)
1 000.0	6.693 9(44)	2.780 180(82)	2.008 11(4)	1.734 6(77)
10 000.0	14.397(8)	4.907 511(5)	3.145 56(62)	2.511(7)

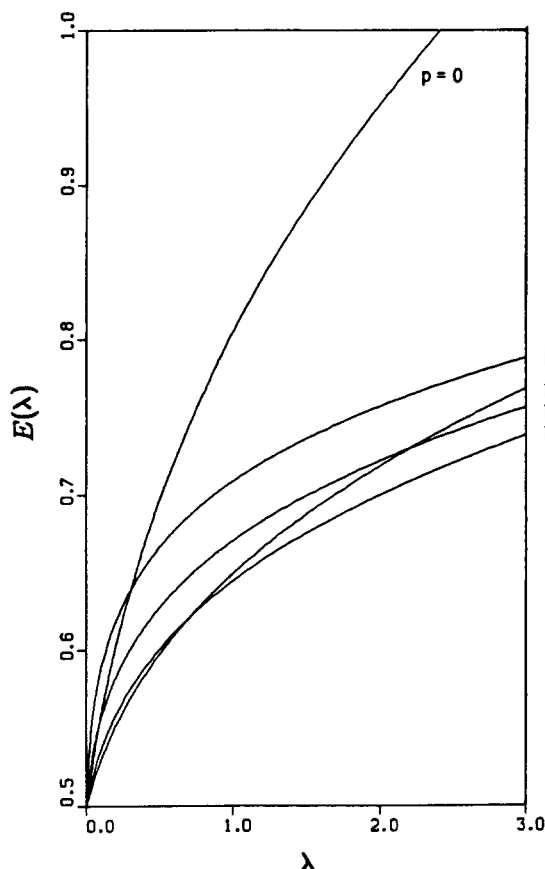


FIG. 1. Ground-state eigenvalues  $E_0^{(p,2)}(\lambda)$  of the generalized one-dimensional quartic anharmonic oscillators defined in Eq. (3.11),  $p = 0, \dots, 4$ .

only for a few specific cases. It is expected, however, that the pattern will appear in general.

The Rayleigh–Schrödinger eigenvalue expansions associated with these radial Hamiltonians are easily calculated via the HVHF method. No wave functions need be calculated, and the only input into the algorithm is the unperturbed energy of the eigenstate in question. For hydrogenic problems, the unperturbed continuum states present difficulties for conventional perturbative treatments, which include the method of Surjan and Angyan.<sup>2</sup> The HVHF method avoids these difficulties. Another method of bypassing these problems is the reformulation of hydrogenic eigenvalue equations by means of a specific realization of the so(4,2) Lie algebra.<sup>41–43</sup> This method is certainly feasible for the hydrogenic problems discussed in Sec. IV. However, the reformulated equation is equivalent to a perturbation problem defined over a nonorthogonal basis set. As such, it would introduce some additional complications into the Surjan–Angyan formulas.

Also, the methods employed here could be applied to more realistic and complicated situations, for example, non-radial perturbations where  $\hat{A}$  and  $\hat{B}$  in Eq. (1.3) represent the dipole moment operator. A so(4,2) Lie algebraic treatment of such problems would be quite straightforward, being similar to the Zeeman and Stark effects which have already been studied in this way.<sup>42,44</sup> A HVHF approach

would involve a coupled system of equations, similar in basic form to that encountered in the Stark effect.<sup>14</sup>

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