RAYLEIGH–SCHRÖDINGER PERTURBATION THEORY AT LARGE ORDER FOR RADIAL RELATIVISTIC HAMILTONIANS USING HYPERVIRIAL AND HELLMANN–FEYNMAN THEOREMS

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Relativistic hypervirial and Hellmann–Feynman theorems are used to construct Rayleigh–Schrödinger expansions for eigenvalues of perturbed radial Dirac equations to aribitrary order. The method is very simple and flexible, requiring no matrix elements. Only the unperturbed energy is required as input. Any difficulties due to the presence of unperturbed continuum states are bypassed. Particular attention is paid to hydrogenic atoms with confining scalar potentials of the form $W(r)=\lambda r^q$, $q=0, 1, 2, \ldots$. Continued fraction representations of these expansions reveal their Stieltjes behavior for $q \geqslant 1$ and Padé summability for $q=1, 2$.

1. Introduction

In this report we outline an effective application of relativistic hypervirial (HV) and Hellmann–Feynman (HF) theorems to calculate Rayleigh–Schrödinger (RS) eigenvalue expansions

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

to arbitrary order in the coupling constant λ for perturbed radial Dirac and Klein–Gordon hamiltonians. The former, the focus of this study, will assume the form ($\hbar=c=1$)

$$\hat{H}=-\alpha\hat{p}-\mathrm{i}\alpha\beta K r^{-1}-\beta[m+W(r)]+V(r) . \quad (1)$$

Here, α and β denote 2×2 matrix operators (see, for example, ref. [1], p. 334 [#1]) satisfying the relations $\alpha^2=\beta^2=I$ (identity), $\alpha\beta+\beta\alpha=0$, and $K=l(l+1)-j(j+1)-\frac{1}{4}=-1, -2, \ldots$, where j and l are the total and orbital angular momentum numbers, respectively. Such hamiltonians have received much attention in the context of quark confinement [2,3] as well as atomic physics [4–7]. The scalar potential $W(r)$ which transforms as the mass, or the external vector potential $V(r)$ (or both) may contain the coupling constant λ which will serve as the RS expansion parameter. An immediate advantage of the HVHF perturbative method is that no matrix elements need be calculated, with only the unperturbed eigenvalue $E^{(0)}$ as input. It is very simple, flexible and readily adapted for either numerical or symbolic computation.

The HF [7] and HV [8] theorems are well known for nonrelativistic hamiltonians and the associated HVHF perturbative method is well established in this domain [9–11]. In the case of hydrogenic problems, the usual difficulties posed by the presence of the unperturbed continuum are bypassed. A number of perturbative methods for relativistic problems have been imported from nonrelativistic theory, including logarithmic perturbation theory [12] and a reformulation [5] over a sturmian-type basis (related, in fact, to the SO(4,2) dynamical group structure of the Dirac hydrogen atom). This, however, has not been the case for the HVHF method. Interestingly enough, the relativistic virial [13] and Hellmann–Feynman [14] theorems for the Dirac and Klein–Gordon equations have been known for some time.

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[#1] We have adopted this older notation to be consistent with the presentations in refs. [4–6] and especially ref. [14], which motivated this work.

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As well, the hypervirial relations for these hamiltonians as applied to hydrogen have been derived explicitly [15,16]. However, these results, slightly more complicated for the spinorial Dirac case, appear never to have been generalized to arbitrary hamiltonians or integrated to develop a relativistic perturbation theory. This task is outline below for the Dirac equation: the Klein–Gordon case will be reported elsewhere. Our goal is to investigate the large order behavior of RS expansions associated with relativistic hamiltonians. The motivation lies in the wealth of information which is contained in the typically divergent expansions encountered in nonrelativistic problems [17]. A further feature is that, in many cases, excellent numerical approximations to eigenvalues may be achieved by appropriate summability techniques.

2. Hypervirial relations

The essence of the HV theorem, relativistic or nonrelativistic, is as follows, Let $\hat{H}$ denote a linear operator, self-adjoint on a Hilbert space $\mathscr{H}$, with eigenvalues given by $\hat{H}\phi_n = E_n\phi_n$, $n=0, 1, 2, \ldots$. The self-adjointness ensures that for any linear operator $\hat{O}$, the following expectation values (suitably defined in $\mathscr{H}$) vanish:

$$\langle [\hat{O}, \hat{H}] \rangle_n \equiv \langle \phi_n | [\hat{O}, \hat{H}] | \phi_n \rangle = 0, \quad n=0, 1, 2, \ldots , \tag{2}$$

where $[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$. When $\hat{O} = \boldsymbol{r}\cdot\boldsymbol{p}$, the relations implied by (2) constitute the quantum mechanical virial theorem. If we let $\hat{O}$ represent the radial operators given below at the left, then the corresponding Dirac hypervirial relations are obtained for $k=0$, 1, 2, ... (omitting the subscript n for convenience):

$$\hat{O} = r^k: \quad k\langle \alpha r^{k-1} \rangle = 0 , \tag{3}$$

$$\hat{O} = \alpha r^k: \quad m\langle \mathrm{i}\alpha\beta r^k \rangle = K\langle \beta r^{k-1} \rangle + \tfrac{1}{2}k\langle r^{k-1} \rangle - \langle \mathrm{i}\alpha\beta r^k W \rangle , \tag{4}$$

$$\hat{O} = r^{k+1}p: \quad m\langle \beta r^k \rangle + E\langle r^k \rangle = \langle r^k V \rangle - \langle \beta r^k W \rangle + \frac{1}{k+1}[\langle r^{k+1}\mathrm{d}V/\mathrm{d}r \rangle - \langle \beta r^{k+1}\mathrm{d}W/\mathrm{d}r \rangle - kK\langle \mathrm{i}\alpha\beta r^{k-1} \rangle] , \tag{5}$$

$$\hat{O} = \beta r^k: \quad E\langle \beta r^k \rangle + m\langle r^k \rangle = \tfrac{1}{2}k\langle \mathrm{i}\alpha\beta r^{k-1} \rangle + \langle \beta r^k V \rangle - \langle r^k W \rangle , \tag{6}$$

$$\hat{O} = \mathrm{i}\alpha\beta r^k: \quad E\langle \mathrm{i}\alpha\beta r^k \rangle + K\langle r^{k-1} \rangle - \langle \mathrm{i}\alpha\beta r^k V \rangle + \tfrac{1}{2}k\langle \beta r^{k-1} \rangle = 0 . \tag{7}$$

Eqs. (3)–(7) represent generalizations of, respectively, eqs. (8), (10), (9), (11) and (12) (for hydrogen) in ref. [15]. The presence of the Dirac matrices produces three sets of expectation values

$$A_k \equiv \langle \mathrm{i}\alpha\beta r^k \rangle, \quad B_k \equiv \langle \beta r^k \rangle, \quad C_k \equiv \langle r^k \rangle , \tag{8}$$

associated with a given eigenstate ϕ_n of eigenvalue E_n. Normalization of ϕ_n requires that $C_0 = 1$. Eqs. (4)–(6) are sufficient for the perturbative methods to be discussed below. They have been written in a form somewhat different to that in ref. [15], in order to reveal a recursive procedure by which the expectation values in (8) may be calculated. We illustrate this method in the case of Dirac hydrogenic atoms, where $W(r)=0$, $m=1$ (atomic units), $V(r) = -\alpha_v r^{-1}$ ($\alpha_v = Z\alpha$ where Z=atomic number, $\alpha \approx 1/137$). This standard problem is, of course, solvable by a differential equation approach [1] as well as by the use of the so(2,1) spectrum generating Lie algebra [18]. The (positive) eigenvalues are given by

$$E = E^{(0)} = [1 + \alpha_v^2/(N - J - \tfrac{1}{2} + \gamma)]^{-1/2} , \tag{9}$$

where $\gamma = [(J+\frac{1}{2})^2 - \alpha_v^2]^{1/2}$, $N = 1, 2, \ldots$ and $J = \frac{1}{2}, \frac{3}{2}, \ldots, N - \frac{1}{2}$. Again, normalization dictates that $C_0 = 1$. Then, $k=0$ in eq. (5) implies $B_0 = \langle \beta \rangle = -E$; $k=0$ in eq. (6) implies $B_{-1} = \langle \beta r^{-1} \rangle = \alpha_v^{-1}(E^2 - 1)$, and $k=0$ in eq. (4) implies $A_0 = K\alpha_v^{-1}(E^2 - 1)$. The elements may now be calculated recursively: (a) set $k=1$, (b) calculate A_k from eq. (4) and B_k, C_k by solving the system of two linear equations (5) and (6) with determinant $\Delta = m^2 - E^2$, (c) increase k by 1 and return to (b). For most hydrogenic perturbation problems this method of initialization and recursion is sufficient and A_{-1}, C_{-1} are not required.

3. Perturbative method and the Hellmann–Feynman theorem

In order to treat perturbation problems (assuming

of course, a solvable unperturbed problem) the essence of the HVHF method is to assume series expansions for the expectation values in eq. (8), i.e.

$$A_k(\lambda)=\sum_{n=0}^{\infty} a_k^{(n)}\lambda^n,\quad B_k(\lambda)=\sum_{n=0}^{\infty} b_k^{(n)}\lambda^n,$$

$$C_k(\lambda)=\sum_{n=0}^{\infty} c_k^{(n)}\lambda^n, \tag{10}$$

with $c_0^{(n)}=\delta_{0n}$ (normalization), as well as the usual RS expansion for the eigenvalue $E(\lambda)$. Formally, the above expansions may be viewed as arising from the usual RS expansion for the wavefunction ψ, which will remain "unseen". The "unperturbed" vectors $\boldsymbol{A}_k(0)$, $\boldsymbol{B}_k(0)$, $\boldsymbol{C}_k(0)$ (i.e. the elements in eq. (8)) now define the first columns of three respective matrices associated with the perturbed problem. In general, eqs. (4)–(6) dictate a set of difference equations which permit a recursive calculation for (i) $a_k^{(n)}$ then (ii) $b_k^{(n)}$ and $c_k^{(n)}$, in a columnwise manner. These coefficients will be related to the RS coefficients $E^{(n)}$ by the appropriate Hellmann–Feynman relation [14]

$$\mathrm{d}E/\mathrm{d}\lambda=\langle \partial H/\partial\lambda\rangle\,. \tag{11}$$

A knowledge of n columns (i.e. nth order perturbation theory) permits the calculation of $E^{(n+1)}$.

4. RSPT and continued fractions at large order

Many nonrelativistic quantum mechanical hamiltonians yield divergent RS expansions whose coefficients grow generically as

$$E^{(n)}\sim(-1)^{n+1}A\Gamma(pn+a)B^n,\quad n\to\infty\,, \tag{12}$$

where $p=1, 2, 3, \ldots$ and A, a and B are constants which have quantum number dependence. Also of interest are the continued fraction (CF) representations [19] of these series,

$$E(\lambda)=E^{(0)}+\lambda C(\lambda)\,, \tag{13a}$$

$$C(\lambda)=\frac{c_1}{1+}\,\frac{c_2\lambda}{1+}\,\frac{c_3\lambda}{1+}\cdots\,. \tag{13b}$$

Many RS expansions are negative Stieltjes for $n\geqslant 1$ [20], in which case $C(\lambda)$ is an S-fraction, i.e. $c_n>0$ for *all* $n\geqslant 1$. There is a general relationship [21] between the large order behavior of Stieltjes perturbation coefficients and their CF counterparts: if the $E^{(n)}$ behave asymptotically as in eq. (12), then

$$c_n=\mathrm{O}(n^p),\quad n\to\infty\,. \tag{14a}$$

In the special case $p=1$, we find, more precisely,

$$c_n\sim\tfrac{1}{2}Bn+A^{(i)}+R_n^{(i)},\quad i=1\ (2),\ n\text{ even (odd)}\,. \tag{14b}$$

The $A^{(i)}$ are constants and $R_n^{(i)}=\mathrm{o}(1)$ as $n\to\infty$.

5. Applications

We first consider the addition of scalar potentials of the form $W(r)=\lambda r^q$, $q=0, 1, 2, \ldots$ to the Dirac hydrogenic atoms defined earlier. Such potentials are known to support bound states and have been considered as models for quark confinement [2,3]. The recursion relations associated with eqs. (4)–(6) and (10) become, respectively,

$$ma_k^{(n)}=Kb_{k-1}^{(n)}+\tfrac{1}{2}kc_{k-1}^{(n)}-a_{k+q}^{(n-1)}\,, \tag{15a}$$

$$mb_k^{(n)}+E^{(0)}c_k^{(n)}=-\frac{k}{k+1}(Ka_{k-1}^{(n)}+\alpha_{\mathrm{v}}c_{k-1}^{(n)})$$
$$-\frac{k+1+q}{k+1}\,b_{k+q}^{(n-1)}-\sum_{j=1}^{n}E^{(j)}c_k^{(n-j)}\,, \tag{15b}$$

$$E^{(0)}b_k^{(n)}+mc_k^{(n)}=\tfrac{1}{2}ka_{k-1}^{(n)}-\alpha_{\mathrm{v}}b_{k-1}^{(n)}$$
$$-c_{k+q}^{(n-1)}-\sum_{j=1}^{n}E^{(j)}b_k^{(n-j)}\,. \tag{15c}$$

From the Hellmann–Feynman theorem, we have $\mathrm{d}E/\mathrm{d}\lambda=-\langle\beta r^q\rangle$. Formal differentiation and matching of asymptotic terms in this equation yields $E^{(n+1)}=-b_p^{(n)}/(n+1)$. In order to determine $E^{(N+1)}$, $N\geqslant 0$, we must calculate the elements of the nth column $a_k^{(n)}$, $b_k^{(n)}$, $c_k^{(n)}$ for $0\leqslant k\leqslant(N+1-n)q$, as well as $b_{-1}^{(n)}$, where $n=0, 1, \ldots, N$. Each new column is initialized as for the unperturbed case: $k=0$ in eq. (15b) gives $b_0^{(n)}$, $k=0$ in eq. (15c) gives $b_{-1}^{(n)}$ and $k=0$ in eq. (15a) gives $a_0^{(n)}$. The symbolic computation language MAPLE [22] has been used for computer calculation of explicit algebraic expressions for the $E^{(n)}$. For example, when $q=1$, the first order RS coefficient is given by

$$E^{(1)}=-\frac{K(Km+E^{(0)})}{2\alpha_{\mathrm{v}}m^2}+\frac{\alpha_{\mathrm{v}}[m^2+2(E^{(0)})^2]}{2m[m^2-(E^{(0)})^2]}\,.$$

Table 1
Estimates of ground state ($N=1, J=1/2, K=-1$) eigenvalues $E(\lambda)$ of the radial Dirac hamiltonian in eq. (1) for $V(r)=-\alpha_v/r$, $W(r)=\lambda r$, $m=1$. The entries represent the lower bounds afforded by the [24,25] (λ) Padé approximant (40th order RSPT) to the RS series for $E(\lambda)$. The upper bounds yielded by the [24,24] (λ) Padé are found by replacing the final n digits in each entry with the n digits in accompanying parentheses.

λ	$\alpha_v=0.9$	$\alpha_v=0.7$	$\alpha_v=0.5$
0.0	0.435889894354067355	0.7141284285428	0.86602540378
0.1	0.474834887551530724(5)	0.810399289403(6)	1.0236814(5)
0.2	0.50627537741 36(7)	0.881838754(61)	1.13113(5)
0.3	0.53354256948(51)	0.9419175(8)	1.2194(6)
0.4	0.55809967(75)	0.994918(21)	1.2963(70)
0.5	0.580419033(40)	1.04293(4)	1.365(7)
1.0	0.673560(2)	1.2388(92)	1.64(6)
2.0	0.8126(8)	1.523(32)	1.98(2.13)
5.0	1.096(103)	2.05(18)	2.5(3.4)

In the rather trivial case $q=0$, we find, as expected, that $E^{(1)}=E^{(0)}$ and $E^{(n)}=0$ for $n\geq 2$. The HVHF method is also applicable to the special case $q=-1$, where $W(r)$ defines an attractive scalar Coulomb-type potential. In this case, the eigenvalues are known in closed form [2,4]. These hamiltonians and their perturbations are discussed in the appendix.

We now consider the large order behavior and summability properties of RS expansions for the cases $q\geq 1$. Without loss of generality, we set $m=1$: a (unitary) scaling transformation $r\to\gamma r$, $\gamma>0$, shows that $E(m,\lambda)=m^{-1}E(1,\lambda m^{-(q+1)})$. For $q=1$, 2, and 3, the RS expansions for ground and several excited states have been calculated to at least order $n=50$ for a number of values of the Coulomb coupling constant α_v. Furthermore, the CF coefficients c_n have also been calculated accurately to this high order. A numerical asymptotic analysis of the coefficients, using a Thiele-continued fraction interpolation scheme [23], reveals the following significant behavior: (i) the $E^{(n)}$ behave asymptotically as in eq. (12), with $p=q$, and (ii) in all cases $C(\lambda)$ is an S-fraction, and the c_n grow as n^q, in accordance with eq. (14).

These observations lead us to conjecture that the RS expansions associated with these scalar perturbations are Stieltjes for all $q\geq 1$. On the basis of the asymptotic behavior of the $E^{(n)}$ and/or the c_n, and Carleman's condition [19], the RS expansions are Padé summable only for $q=1$, 2. This behavior is quite analogous to the case of nonrelativistic hydrogenic atoms perturbed by radial potentials of the form λr^q [24]. In table 1 are presented the lower and upper bounds to $E(\lambda)$ for the case $q=1$ (linear confining potential) yielded by, respectively, [25,25] and [24,25] Padé approximants to the RS series, for several values of α_v. These approximants are obtained from appropriate truncations of $C(\lambda)$ [19,23]. The bounds are consistent with numerical estimates obtained by the eigenvalue search algorithm described in ref. [2] (eqs. (21)–(28)). In table 2 are presented some bounds for the first excited state eigenvalues. For a given order, the accuracy of the Padé method is seen to decrease with a decrease with a decrease in α_v. This is consistent with the observation that the geometric divergence of the $E^{(n)}$, i.e. the factor B in eq. (12), is proportional to an inverse power of α_v. A future report will deal with analytic expressions for the large order behavior of the $E^{(n)}$.

6. Vector potentials

We now consider perturbations to the vector Coulomb potential of hydrogenlike atoms. $V(r)=-\alpha_v r^{-1}+\lambda r^p$, $\alpha_v>0$, $p=0, 1, 2, \ldots$. The recursion relations for the HV coefficients have essentially the same form as eq. (15), except that we (i) remove the final term from eq. (15a) and modify appropriately the penultimate terms in eqs. (15b), (15c). Only the case $p=1$ has been investigated in some detail. The $E^{(n)}$ alternate in sign and diverge. However, the CF representations are not Stieltjes, since there are regular periodic "eruptions" where the c_n assume negative values. This implies that some

Table 2
Bounds for first excited state eigenvalues ($N=1, J=1/2, K=-1$).

λ	$\alpha_v=0.9$	$\alpha_v=0.7$	$\alpha_v=0.5$
0.0	0.84731632	0.925815	0.965925
0.1	1.0948312(3)	1.2717(8)	1.390(7)
0.2	1.260125(42)	1.4836(62)	1.613(71)
0.3	1.3949(51)	1.650(62)	1.77(92)
0.4	1.5117(25)	1.79(82)	1.9(2.2)
0.5	1.6161(83)	1.91(6)	2.0(2.4)

Padé approximants may have poles on the positive real line, affecting convergence. The non-Stieltjes behavior of these cases may be related to a "Klein paradox" for such potentials [25].

This example is quite easily extended to the problem of hydrogenic atoms with screened Coulomb potentials of the form [5,6]

$$V(r)=-\frac{\alpha_v}{r}\sum_{j=0}^{\infty} v_j\lambda^j r^j, \quad v_0=1,$$

involving some modifications of eqs. (15b), (15c). The results agree with those given in refs. [5] and [6] (reported to 3rd and 5th order, respectively). (The HVHF treatment of the nonrelativistic version of this problem is described in ref. [26].) For the particular case of a Yukawa potential, i.e. $v_j=(-1)^j/j!$, the CF representations exhibit the periodic "negative eruptions" described above. $C(\lambda)$ cannot represent a Stieltjes function, since this potential supports each bound state only to its coupling constant threshold, i.e., i.e. for $0<\lambda<\lambda^*$. However, excellent estimates to $E(\lambda)$ in this region are obtained from Padé approximants whose poles lie away from the positive real line. This situation is also observed for the corresponding nonrelativistic Yukawa problem [27].

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Appendix

A set of more complicated problems involves perturbations of the solvable Dirac hamiltonians defined by the potentials $W(r)=-\alpha_s/r$, $V(r)=-\alpha_v/r$, where $\alpha_v>0$. The parameter α_s represents a scalar coupling constant. The positive eigenvalues of this hamiltonian are given by [2,3]

$$E(\alpha_v,\alpha_s)=\frac{-\alpha_v\alpha_s+(n+g)[(n+g)^2+\alpha_v^2-\alpha_s^2]^{1/2}}{(n+g)^2+\alpha_v^2}, \quad (A.1)$$

where $n=N-J-\frac{1}{2}$ is the radial quantum number and $g=(K^2+\alpha_s^2-\alpha_v^2)^{1/2}$. The scalar potential $m+W(r)$ may be interpreted asa coordinate dependent mass. Such hamiltonians have also been discussed in the context of muonic effects in atoms [3] as well as in quark-confinement models [2]. In the special case $\alpha_v=\alpha_s$, the eigenvalues in (A.1) have been shown to be eigenvalues of a slightly "renormalized" Schrödinger wave equation [28].

The presence of the $1/r$ term in $W(r)$ slightly complicates the RS procedure: the terms $a_{-1}^{(n)}$ and $c_{-1}^{(n)}$ must now be calculated for all $n\geq 0$. However, these values are available from appropriate Hellmann–Feynman expressions. The RS coefficients $E^{(n)}$ may be considered as functions of the parameters N, K, α_v and α_s. Termwise partial differentiation of the asymptotic RS expansion for $E(\lambda)$ in terms of these parameters is justified [29], yielding the relations

$$a_{-1}^{(n)}=-\frac{\partial E^{(n)}}{\partial K}, \quad c_{-1}^{(n)}=-\frac{\partial E^{(n)}}{\partial \alpha_v},$$

$$b_{-1}^{(n)}=-\frac{\partial E^{(n)}}{\partial \alpha_s}. \quad (A.2)$$

Of course, these differentiations must be performed algebraically, for which the MAPLE symbolic manipulation language has been used. This represents a greater computational requirement, however, since the complexity of the algebraic expressions grows rapidly with the repeated differentiation.

When the scalar term α_s/r is treated as a perturbation of a Dirac hydrogenic atom, i.e. the case $q=-1$ of the main text, this method yields an α_s series which is identical to that obtained by expanding

eq. (A.1) as a Taylor series in α_s. Other problems have been considered, including "screened" scalar and vector Coulomb potentials, but will have to be discussed elsewhere.

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