Rayleigh-Schrödinger perturbation theory at large order for radial Klein-Gordon equations

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The relativistic hypervirial and Hellmann-Feynman theorems for the Klein-Gordon (KG) equation are used to construct Rayleigh-Schrödinger (RS) perturbation expansions to arbitrary order. The method is applied to the KG equation for a particle in an attractive Coulomb-type vector potential with perturbing vector or scalar potentials of the form λr^k, $k=1,2,\ldots$. In the scalar case, such potentials are confining and the RS expansions exhibit Stieltjes behavior for $k\geq 1$ and Padé summability for $k=1,2$.

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I. INTRODUCTION

This paper is concerned with Rayleigh-Schrödinger (RS) perturbation expansions of three-dimensional Klein-Gordon (KG) equations with radially symmetric potentials. If $\psi(\mathbf{r})$ denotes the wave function of the KG particle, a separation of variables $\psi(\mathbf{r})=r^{-1}R(r)Y(\theta,\phi)$ yields the following radial equation (in units $\hbar=c=1$):

$$\hat{F}R(r)=\left[-\frac{d^2}{dr^2}+\frac{L(L+1)}{r^2}+[m+W(r)]^2 -[E-V(r)]^2\right]R(r)=0 , \qquad (1.1)$$

where $\hat{D}\equiv d/dr$, E is the energy, L is the angular momentum, $V(r)$ is the vector potential, and $W(r)$ is the scalar potential. Dirac and Klein-Gordon equations with vector and/or scalar potentials have received attention as possible models of quark confinement.

In particular, we shall focus on perturbations of a Klein-Gordon particle in a Coulomb-type vector potential, i.e., $W(r)=0$ and $V(r)=-Z/r$, where Z represents an effective field strength. This solution to this problem, the so-called *π-mesonic atom* [1], is well known: the eigenvalues are given by [2]

$$E=E_{NL}^{(0)} =m\left[1+\frac{Z^2}{\{[N_r+\frac{1}{2}]+[(L+\frac{1}{2})^2-Z^2]^{1/2}\}^2}\right]^{-1/2} , \qquad (1.2)$$

where N_r, $L=0,1,2,\ldots$, are the radial and angular quantum numbers, respectively, and $N=N_r+L+1$ is the principal quantum number. (In this paper, uppercase indices will be reserved for quantum numbers.) The perturbations to the above potentials will have the form λr^k, $k=1,2,\ldots$, where λ represents the perturbation parameter. The relativistic hypervirial (HV) and Hellmann-Feynman (HF) theorems for the KG equation will then be used to generate RS perturbation expansions for the eigenvalue

$$E_{NL}(\lambda)=\sum_{n=0}^{\infty}E_{NL}^{(n)}\lambda^n . \qquad (1.3)$$

The large-order behavior of the RS coefficients as well as the summability properties of the series in (1.3) will be of interest.

The use of nonrelativistic HV and HF theorems to generate quantum-mechanical perturbation expansions is well known [3,4] (see Ref. [5] for a comprehensive review). There are several advantages to this method: no wave functions or matrix elements need to be calculated and in the case of hydrogenic perturbation problems, difficulties due to the presence of the unperturbed continuum states are avoided. The relativistic versions of the HV and HF theorems for Dirac and Klein-Gordon equations have been known for some time [6–9]. However, their application to perturbed relativistic problems, namely the Dirac case, has been reported only quite recently [10]. This paper represents the completion of our study of relativistic problems. (A similar situation exists for the classical HV and HF theorems. It was recently shown [11] that these theorems may also be used to generate perturbation expansions for classical periodic orbits of integrable systems. The expansions which are obtained coincide with the results of canonical or Poincaré–von Zeipel perturbation theory.)

A number of other perturbation methods have been developed for the KG equation, including logarithmic perturbation theory [12] and $1/N$ expansions [13]. For radial potentials, the KG equation may also be rewritten in terms of the elements of an so(2,1) Lie algebra [14] and, as in the nonrelativistic case [15], a perturbation theory may be formulated. However, this method is extremely tedious for relativistic problems [16]. In comparison, the HVHF method will be seen to yield an extremely simple perturbation method.

It is interesting to note that a closed-form solution to the KG equation also exists in the case that *both* $V(r)$ and $W(r)$ in (1.1) are attractive Coulomb-type potentials. Such explicit solutions are known for the Dirac equation

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[17, Sec. 3.4] but, to the best of our knowledge, have not been reported for the KG equation. We include a brief derivation of this simple result in the Appendix.

In Sec. II, the hypervirial and Hellmann-Feynman theorems for the KG equation are presented along with a description of the HVHF perturbative method. In Sec. III, the method is applied to radial vector and scalar perturbations of the π-mesonic atom described above. Algebraic computations have been performed using the computer-algebra language MAPLE [18].

II. HYPERVIRIAL AND HELLMANN-FEYNMAN THEOREMS FOR THE KG EQUATION AND PERTURBATION THEORY AT LARGE ORDER

In this section, we review the HV and HF theorems for the KG equation and introduce the associated HVHF perturbation method. The HVHF method involves expectation values of operators. Since only radially symmetric problems are considered here, all relevant operators will act only on the radial coordinate r. Given a radial operator $\hat{O}$, its expectation value with respect to the radial wave function $R(r)$ will be denoted as

$$\langle \hat{O} \rangle \equiv \int_0^\infty \bar{R}(r)\hat{O}R(r)dr \ . \tag{2.1}$$

As such, we consider the operator $\hat{O}$ [as well as $\hat{F}$ in (1.1)] to be self-adjoint on the Hilbert space $\mathcal{H}=L^2([0,\infty),dr)$.

Because of the quadratic nature of the KG equation in (1.1), the HV and HF relations for specific problems are more complicated than their nonrelativistic counterparts.

A. KG hypervirial theorem [9]

Assume that $\psi=r^{-1}R(r)Y(\theta,\phi)$ is a solution to Eq. (1.1) and that $\hat{O}$ is self-adjoint on $\mathcal{H}$. Then

$$\langle [\hat{O},\hat{F}] \rangle = 0 \ . \tag{2.2}$$

where $[\hat{A},\hat{B}]=\hat{A}\hat{B}-\hat{B}\hat{A}$.

If we now choose $\hat{O}=r^k\hat{D}$, $k\in\mathbb{Z}$, where $\hat{D}\equiv d/dr$, a set of recursion relations involving the expectation values $\langle r^k\rangle=\int_0^\infty \bar{R}r^kR\,dr$ is obtained. These are known as the *hypervirial relations*. The following relations are needed for the evaluation of the commutator in (2.2):

$$[\hat{D},\hat{F}]=-\frac{2L^2}{r^3}+2E(\hat{D}V)-2V(\hat{D}V) \ , \tag{2.3a}$$

$$[r^k,\hat{F}]=2kr^{k-1}\hat{D}+k(k-1)r^{k-2} \ , k\in\mathbb{Z} \ , \tag{2.3b}$$

where $(\hat{D}V)\equiv dV/dr$. Using the identity $[r^k\hat{D},\hat{F}]=r^k[\hat{D},\hat{F}]+[r^k,\hat{F}]\hat{D}$, all appearances of $\hat{D}$ and $\hat{D}^2$ are eliminated. Taking expectation values with respect to the radial solution R with corresponding energy E yields the HV relations.

For the KG equation in (1.1), the HV relations are given by

$$k[L^2-\tfrac{1}{4}(k^2-1)]\langle r^{k-2}\rangle+E\langle r^{k+1}(\hat{D}V)\rangle+m\langle r^{k+1}(\hat{D}W)\rangle+\langle r^{k+1}W(\hat{D}W)\rangle-\langle r^{k+1}V(\hat{D}V)\rangle$$
$$+2(k+1)E\langle r^kV\rangle+2(k+1)m\langle r^kW\rangle+(k+1)(m^2-E^2)\langle r^k\rangle+(k+1)\langle r^kW^2\rangle-(k+1)\langle r^kV^2\rangle=0 \ . \tag{2.4}$$

For the particular case of an attractive Coulombic-type scalar potential, i.e., the π-mesonic atom, $V(r)=-Z/r$, the HV relations yield a recursion relation for the expectation values $\langle r^k\rangle$:

$$\begin{aligned}(k+1)[E^2-m^2]\langle r^k\rangle &= k[L(L+1)-Z^2-\tfrac{1}{4}(k^2-1)]\langle r^{k-2}\rangle \\ &\quad -(2k+1)ZE\langle r^{k-1}\rangle \ ,\end{aligned} \tag{2.5}$$

where E is given in Eq. (1.2). This is the result obtained by Epstein [Ref. [9], Eq. (6)]. Equation (2.5) can also be rearranged to compute (nonsingular) expectation values of inverse powers of r as well. Some expectation values are given in Table I.

B. KG Hellmann-Feynman theorem [9]

Assume that the KG operator $\hat{F}$ in Eq. (1.1) contains a scalar parameter λ and that the operator $\partial\hat{F}/\partial\lambda$ is also self-adjoint in $\mathcal{H}$. Then, for a solution ψ,

$$\left\langle \frac{\partial \hat{F}}{\partial\lambda} \right\rangle = 0 \ . \tag{2.6}$$

Now assume that the explicit λ dependence of $\hat{F}$ is contained in the potentials V and W. Furthermore, consider the energy E to be an implicit function of λ. Then, from Eq. (2.6),

$$\left\langle (m+W)\frac{\partial W}{\partial\lambda}-(E-V)\left[\frac{\partial E}{\partial\lambda}-\frac{\partial V}{\partial\lambda}\right]\right\rangle = 0 \tag{2.7}$$

TABLE I. Some expectation values $\langle r^k\rangle$ for the solutions of the unperturbed Klein-Gordon equation (1.1) for the π-mesonic atom, with $W(r)=0$ and $V(r)=-Z/r$. Here $K^2=L(L+1)$ and the energy E is given in Eq. (1.2).

k	$\langle r^k\rangle$
-1	$-\frac{1}{ZE}(E^2-m^2)$
0	1
1	$-\frac{1}{2ZE}(K^4E^2-m^2K^4-2Z^2K^2E^2$ $+m^2Z^2K^2+Z^4E^2-m^2Z^4+3Z^2E^2)$
2	$\frac{1}{6}(4K^4-8Z^2K^2+4Z^4-3+5K^4E^2-5m^2K^4$ $-10Z^2K^2E^2+10m^2Z^2K^2+5Z^4E^2-5m^2Z^4+15Z^2E^2)$

or

$$m\left\langle\frac{\partial W}{\partial\lambda}\right\rangle+\left\langle W\frac{\partial W}{\partial\lambda}\right\rangle-E\frac{\partial E}{\partial\lambda}+\langle V\rangle\frac{\partial E}{\partial\lambda}+E\left\langle\frac{\partial V}{\partial\lambda}\right\rangle-\left\langle V\frac{\partial V}{\partial\lambda}\right\rangle=0\ . \tag{2.8}$$

C. HVHF perturbative method

For perturbation problems where the potentials contain a perturbation parameter λ, the HV relations will necessarily include powers of λ. As in the nonrelativistic case, the essence of the HVHF perturbative method is to assume the following perturbation expansions for a given state ψ with energy E (for simplicity of notation, quantum number indices will be suppressed):

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

$$\langle r^k\rangle=\sum_{n=0}^{\infty}C_k^{(n)}\lambda^n\ . \tag{2.9b}$$

The normalization condition $\langle r^0\rangle=1$ implies that

$$C_0^{(0)}=1\ ,\quad C_0^{(n)}=0\ ,\quad n\geq 1\ . \tag{2.10}$$

Substitution of these expansions into the HV relations and collection of terms in λ^n yields a set of relations involving the coefficients $E^{(n)}$ and $C_k^{(n)}$. However, the HV relations themselves are not closed. The Hellmann-Feynman theorem provides the relationship between the $C_k^{(n)}$ and the $E^{(n)}$. [In most cases, the RS perturbation series for $E(\lambda)$ is at least asymptotic over an appropriate sector of the complex-λ plane, and termwise differentiation is permitted.] As in the nonrelativistic case, the **C** array is generally calculated columnwise, starting with the unperturbed column $C_k^{(0)}$ which, as in standard perturbation theory, is assumed to be known. A knowledge of the nth column of the table permits the computation of $E^{(n+1)}$.

In addition to the RS expansions for these problems, we also consider their continued-fraction (CF) representations [19] which have the form

$$E(\lambda)=E^{(0)}+\lambda C(\lambda)\ , \tag{2.11}$$

where

$$C(\lambda)=\frac{c_1}{1+}\frac{c_2\lambda}{1+}\frac{c_3\lambda}{1+}\cdots\ . \tag{2.12}$$

By setting $c_{n+1}=0$, $n=1,2,\ldots$, in Eq. (2.12), one obtains the *convergents* $w_n(z)$ of $C(z)$. The convergents $w_{2n}(z)$ and $w_{2n+1}(z)$ are, respectively, the $[N-1,N]$ and $[N,N]$ Padé approximants [22] to the series for $E(z)$. It is computationally advantageous to generate these diagonal Padé sequences by means of CF's. In many cases, however, there also exists an important relationship [20] between the asymptotics of the CF coefficients c_n and those of the series coefficients $E^{(n)}$, as we briefly review below.

For many standard perturbation problems, e.g., anharmonic oscillators, the RS coefficients $E^{(n)}$ in Eq. (2.9a) behave asymptotically as

$$E^{(n)}\sim(-1)^{n+1}A\,\Gamma(mn+a)b^n\quad\text{as } n\to\infty\ , \tag{2.13}$$

where A, B, a, and b are constants, with $m=1,2,3,\ldots$. In addition, these RS expansions are typically negative Stieltjes for $n\geq 1$ [21], which implies that $C(\lambda)$ in Eq. (2.12) is an S fraction, i.e., all coefficients c_n are positive. When such Stieltjes series coefficients behave asymptotically as in Eq. (2.13), the large-order behavior of the CF coefficients c_n is given by [20]

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

Typically, the $\{c_n\}$ sequence is composed of the two subsequences, $\{c_{n,\text{even}}\}$ and $\{c_{n,\text{odd}}\}$, which exhibit the same dominant behavior but have subdominant corrections with different coefficients. For Stieltjes series, the two (Padé) sequences $\{w_{2n}(z)\}$ and $\{w_{2n+1}(z)\}$ provide, respectively, lower and upper bounds to $E(z)$. If the series is Padé summable [which is guaranteed for $m\leq 2$ in (2.14)], then these sequences converge to $E(z)$ in the limit $n\to\infty$.

In Ref. [10], the RS expansions for Dirac hydrogenic atoms with radial scalar and vector perturbations were studied along with their CF representations. In the case of scalar perturbations of the form $W(r)=\lambda r^q$, $q=1,2,\ldots$, the RS series exhibit Stieltjes behavior. Furthermore, for $q=1,2$, the series are Padé summable. A similar behavior is observed for perturbed Klein-Gordon equations, as will be shown in the next section.

III. SPECIFIC APPLICATION TO PERTURBED HYDROGENIC PROBLEMS

In this section we examine the expansions associated with radial perturbations of the hydrogenic, or π-mesonic atom, whose unperturbed energies are given in Eq. (1.2).

A. Perturbed vector potential

We first consider radial perturbations of the vector Coulombic potential

$$V(r)=-\frac{Z}{r}+\lambda r^p\ ,p=1,2,\ldots\ , \tag{3.1}$$

and $W(r)=0$. Such potentials are not confining potentials: if a Carlini-Liouville-Green-type expansion (see Ref. [23], p. 80) having the form $R(r)\sim e^{S(r)}$ as $r\to\infty$ is assumed, then

$$S(r)\sim\pm\frac{i\lambda r^{p+1}}{p+1}\quad\text{as } r\to\infty\ ,$$

revealing that $R(r)$ is oscillatory.

The hypervirial relations associated with these problems are given by

$$k[L(L+1)-Z^2-\tfrac{1}{4}(k^2-1)]\langle r^{k-2}\rangle-(2k+1)ZE\langle r^{k-1}\rangle+(k+1)(m^2-E^2)\langle r^k\rangle$$
$$+\lambda Z(p+2k+1)\langle r^{k+p-1}\rangle+\lambda(2k+p+2)E\langle r^{k+p}\rangle-\lambda^2(k+p+1)\langle r^{k+2p}\rangle=0\ ,\quad k\in\mathbb{Z}\ , \tag{3.2}$$

and may be compared with their unperturbed counterparts in Eq. (2.5). From Eq. (2.8), the Hellmann-Feynman relations become

$$\lambda\langle r^{2p}\rangle+E\frac{\partial E}{\partial\lambda}+Z\frac{\partial E}{\partial\lambda}\langle r^{-1}\rangle-E\langle r^p\rangle-\lambda\frac{\partial E}{\partial\lambda}\langle r^p\rangle-Z\langle r^{p-1}\rangle=0\ . \tag{3.3}$$

The HF relations provide the following connection between the expansion coefficients for the energy and expectation values (for simplicity of notation, we omit quantum number indices):

$$E^{(n+1)}=\frac{1}{(n+1)(E^{(0)}+ZC_{-1}^{(0)})}\left[-C_{2p}^{(n-1)}+\sum_{i=0}^{n}(i+1)E^{(i)}C_p^{(n-i)}\right.$$
$$\left.+ZC_{p-1}^{(n)}-\sum_{i=0}^{n-1}(i+1)E^{(i+1)}(E^{(n-i)}+ZC_{-1}^{(n-i)})\right]\ ,\quad n=0,1,2,\ldots\ . \tag{3.4}$$

It now remains to find the recursion relations for the $C_k^{(n)}$. Substitution of the expansions in Eq. (2.6) into Eq. (3.2) followed by a rearrangement yields

$$(k+1)[(E^{(0)})^2-m^2]C_k^{(n)}=kC_{k-2}^{(n)}[L(L+1)-Z^2-\tfrac{1}{4}(k^2-1)]-(k+p+1)C_{k+2p}^{(n-2)}$$
$$-Z(2k+1)\sum_{i=0}^{n}E^{(i)}C_{k-1}^{(n-i)}+(2k+p+2)\sum_{i=0}^{n-1}E^{(i)}C_{k+p}^{(n-i+1)}$$
$$+ZC_{k+p-1}^{(n-1)}(2k+p+1)-(k+1)\sum_{i=1}^{n}\sum_{j=0}^{i}E^{(j)}E^{(i-j)}C_k^{(n-i)}\ . \tag{3.5}$$

Equation (3.5) may be used to compute the **C** table columnwise from the unperturbed column $C_k^{(0)}$ [cf. Eq. (2.5) and Table I]. From Eqs. (3.4) and (3.5), it is clear that the expression for $\langle r^{-1}\rangle$ is also required. A rearrangement of Eq. (3.5), with $k=0$, allows the $C_{-1}^{(n)}$ column to be computed separately as follows:

$$C_{-1}^{(n)}=\frac{1}{ZE^{(0)}}\left[-Z\sum_{i=1}^{n}E^{(i)}C_{-1}^{(n-i)}+Z(p+1)C_{p-1}^{(n-1)}-(p+1)C_{2p}^{(n-2)}+(p+2)\sum_{i=0}^{n-1}E^{(i)}C_p^{(n-i-1)}-\sum_{j=0}^{n}E^{(j)}E^{(n-j)}\right]\ . \tag{3.6}$$

For the case $p=1$, i.e., a linear perturbing potential, the first three RS coefficients for the energy E are given in Table II.

For the two cases $p=1,2$, the RS coefficients $E^{(n)}$ as well as their CF counterparts c_n have been computed numerically to large order (i.e., $n\sim100$) for a number of physically allowable values of Z (the mass has been set to $m=1$). In all cases, numerical ratio tests show that the perturbation series are divergent. As well, the c_n begin to grow in a regular fashion but eventually exhibit "eruptions" where large positive and negative values are assumed, followed by regions of rather regular monotonic behavior. The negativity of at least one CF coefficient indicates that the RS series is not Stieltjes. (Note that these eruptions are not due to numerical roundoff errors. The computations were performed using no less than 50 digits of accuracy in MAPLE.) In Table III are listed the first 35 CF coefficients c_n for the particular case $Z=0.5$, $m=1$, $N_r=0$, and $L=0$ as well as the estimates of $E(\lambda)$ for $\lambda=0.5$ provided by the CF convergents $w_n(\lambda)$. For $n<28$, the c_n are positive and the convergents are behaving in a "Stieltjes fashion," i.e., $w_{2k}(\lambda)<w_{2k+1}(\lambda)$ for $k\le13$. As well, the estimates provided by the sequences $\{w_{n,\text{odd}}\}$ and $\{w_{n,\text{even}}\}$ appear to be converging from above and below, respectively, to a common limit. However, at $n=29$, due to the eruption of the c_n, these sequences cross and the roles of odd and even convergents become reversed. For $n>35$, a temporary convergence is again observed until the next eruption of the c_n at $n=48$. Apart from these occasional eruptions, the convergents

TABLE II. Rayleigh-Schrödinger coefficients $E^{(n)}$ for the KG π-mesonic atom with perturbed scalar potential, i.e., $V(r)=-Z/r+\lambda r$ and $W(r)=0$. Here $K^2=L(L+1)$ and the unperturbed energy $E_0=E^{(0)}$ is given in Eq. (1.2).

n	$E^{(n)}$
0	E_0
1	$\dfrac{E_0(3m^2Z^2-m^2K^2+K^2E_0^2)}{2Zm^2(m^2-E_0^2)}$
2	$-\dfrac{E_0}{8m^4Z^2(m^2-E_0^2)^3}(3m^4K^4E_0^2-K^4E_0^6+m^4Z^2E_0^2-6m^6K^2Z^2+12m^6Z^4+2m^6Z^2-2m^6K^4-6m^2K^2Z^2E_0^4-5m^4Z^4E_0^2-3m^2Z^2E_0^4+12m^4K^2Z^2E_0^2)$

$w_n(\lambda)$ are generally hovering about a fixed value. In Table IV are listed the convergents $w_{39}(\lambda)$ and $w_{40}(\lambda)$ for a variety of Z and λ values. Since the potential is not confining, we expect that these values are estimates of the real part of $E(\lambda)$: perturbation theory will not detect the imaginary part which probably vanishes exponentially rapidly as $\lambda \to 0^+$.

B. Perturbed scalar potential — "perturbed mass"

We now consider the π-mesonic atom with radial perturbations to the mass term, i.e.,

$$V(r) = -\frac{Z}{r}\ , \quad W(r) = \lambda r^q\ , \quad q = 1, 2, \ldots\ . \tag{3.7}$$

These scalar potentials are confining: a Carlini-Liouville-Green-type expansion $R(r) \sim e^{S(r)}$ as $r \to \infty$ yields

$$S(r) \sim \pm \frac{\lambda r^{p+1}}{p+1} \quad \text{as } r \to \infty\ ,$$

which indicates that a decaying solution indeed exists.

The perturbation method proceeds in a fashion analogous to that of Sec. III A. The hypervirial relations associated with these problems are given by

$$\begin{aligned} &k[L(L+1) - Z^2 - \tfrac{1}{4}(k^2-1)]\langle r^{k-2}\rangle \\ &\quad -(2k+1)ZE\langle r^{k-1}\rangle + (k+1)[m^2 - E^2]\langle r^k\rangle \\ &\quad + \lambda m(q+2k+2)\langle r^{k+q}\rangle + \lambda^2(k+q+1)\langle r^{k+2q}\rangle = 0 \end{aligned} \tag{3.8}$$

and the Hellmann-Feynman theorem yields

$$m\langle r^q\rangle + \lambda\langle r^{2q}\rangle - E\frac{\partial E}{\partial \lambda} - Z\frac{\partial E}{\partial \lambda}\langle r^{-1}\rangle = 0\ . \tag{3.9}$$

The HF relations imply the following connection between expansion coefficients:

TABLE III. Coefficients c_n of the continued-fraction representation of the RS perturbation series for the ground-state ($N_r = L = 0$) KG π-mesonic atom with $V(r) = -Z/r + \lambda r$, with $Z = 0.5$. The non-Stieltjes nature of the series is revealed by an "eruption" of the c_n at $n = 28, 29, 30$. The final column lists estimates to $E(\lambda)$ for $\lambda = 0.5$, as yielded by the corresponding convergents, i.e., $E^{(0)} + \lambda w_n(\lambda)$.

n	c_n	$E^{(0)} + 0.5 w_n(0.5)$
1	1.060 660 171 7	1.237 436 867 0
2	2.750 000 000 0	0.930 403 659 5
3	6.022 727 272 7	1.102 057 246 0
4	8.164 065 180 1	0.991 711 061 1
5	9.590 147 553 2	1.061 378 088 0
6	11.827 893 854 2	1.013 617 701 4
7	12.890 443 970 4	1.045 598 323 3
8	15.490 381 344 3	1.022 603 627 9
9	16.164 980 389 9	1.038 568 501 2
10	19.250 788 577 9	1.026 652 926 4
11	19.336 352 616 7	1.035 116 929 2
12	23.155 434 534 5	1.028 597 018 3
13	22.347 168 645 0	1.033 288 807 9
14	27.281 251 477 2	1.029 569 469 9
15	25.111 712 740 2	1.032 256 349 8
16	31.749 537 416 1	1.030 066 423 0
17	27.500 569 558 4	1.031 638 283 4
18	36.765 257 740 3	1.030 320 434 0
19	29.301 518 038 3	1.031 246 945 4
20	42.709 535 968 7	1.030 446 638 7
21	30.129 900 775 0	1.030 984 727 8
22	50.407 771 616 1	1.030 504 760 4
23	29.163 332 062 6	1.030 798 335 6
24	62.169 107 914 5	1.030 527 219 7
25	24.104 854 342 3	1.030 657 279 3
26	88.520 951 344 4	1.030 532 632 5
27	4.448 752 384 2	1.030 543 193 9
28	557.432 793 353 6	1.030 532 673 7
29	−457.747 124 069 6	1.030 444 239 5
30	−6.225 894 564 9	1.030 535 800 8
31	112.672 803 584 5	1.030 351 943 2
32	28.777 375 411 8	1.030 549 415 6
33	84.489 886 818 9	1.030 259 158 2
34	43.280 637 201 5	1.030 581 075 5
35	76.863 452 669 2	1.030 158 305 3

TABLE IV. Padé-CF sums of the RS expansions for the energy $E(\lambda)$ of the ground-state ($N_r = L = 0$) Klein-Gordon π-mesonic atom with perturbed scalar potential, i.e., $V(r) = -Z/r + \lambda r$ in Eq (3.7), for various values of Z and λ. Each entry is the convergent $w_{39}(\lambda)$ of the Stieltjes continued-fraction representation (equivalently, the [19,19] Padé approximant) of the RS perturbation series. The convergent $w_{40}(\lambda)$ ([19,20] Padé) is obtained by replacing the final k digits of each entry with the k digits in parentheses.

λ \ Z	0.5	0.4	0.3	0.2
0.0	0.707 106 781 186 54	0.894 427 190 999 91	0.948 683 298 050 51	0.978 906 312 930 70
0.01	0.717 444 184 465 64	0.919 049 561 873 04	0.984 379 538 0 (78)	1.027 622 (19)
0.05	0.754 810 427 923 84	0.997 350 23(19)	1.086 12(08)	1.152(48)
0.1	0.795 714 744 277(07)	1.075 966 6(05)	1.183 98(08)	1.277(48)
0.2	0.866 135 31(67)	1.204 88(59)	1.345(34)	1.50(37)
0.3	0.926 9(68)	1.313 8(20)	1.487(52)	1.73(45)

$$E^{(n+1)}=\frac{1}{(n+1)(ZC_{-1}^{(0)}+E^{(0)})}\left[C_{2q}^{(n-1)}+mC_q^{(n)}-\sum_{i=1}^{n-1}(i+1)E^{(i+1)}(ZC_{-1}^{(n-i)}+E^{(n-i)})\right]. \quad (3.10)$$

The following recursion relations follow from the HV equations:

$$\begin{aligned}(k+1)[(E^{(0)})^2-m^2]C_k^{(n)}=&\,k[L(L+1)-Z^2-\tfrac{1}{4}(k^2-1)]C_{k-2}^{(n)}+(k+q+1)C_{k+2q}^{(n-2)}\\&+m(q+2k+2)C_{k+q}^{(n-1)}-Z(2k+1)\sum_{i=0}^{n}E^{(i)}C_{k-1}^{(n-i)}\\&-(k+1)\sum_{i=1}^{n}\sum_{j=0}^{i}E^{(j)}E^{(i-j)}C_k^{(n-i)},\end{aligned} \quad (3.11)$$

$$C_{-1}^{(n)}=\frac{1}{ZE^{(0)}}\left[-Z\sum_{i=1}^{n}E^{(i)}C_{-1}^{(n-i)}-\sum_{i=0}^{n}E^{(i)}E^{(n-i)}+(q+1)C_{2q}^{(n-2)}+m(q+2)C_q^{(n-1)}\right]. \quad (3.12)$$

(The case $q=0$, which implies a constant shift λ in the mass term and whose solution is hence known, provides a useful check on the validity of the perturbation method.) For the case $q=1$, the first three RS corrections are given in Table V. For the two cases $q=1,2$, the RS coefficients $E^{(n)}$ as well as the CF coefficients c_n have been computed numerically to large order ($n\sim 50$) for a variety of values of Z (again with $m=1$). In all cases, the c_n are positive. As well, difference tables show that the coefficients exhibit a regular growth of the form $c_n\sim O(n^q)$. On the basis of this numerical evidence, we conjecture that this asymptotic behavior exists for $q=1,2,\ldots$ and the RS series is Padé summable for $q=1,2$. For the case $q=1$, estimates of the energy $E(\lambda)$ afforded by the CF convergents for various Z values are presented in Table VI.

The Padé-CF estimates of Tables V were checked by numerical integration of the radial eigenvalue problem. The NAG library subroutine D02KDF, which is designed to treat singular eigenvalue problems, was used: the Klein-Gordon equation is singular at $r=0$ due to the presence of the Coulomb-type potential as well as any angular momentum terms. In general, the results agreed with the Padé sums. The results afforded by numerical integration were extremely sensitive to the choice of the "cutoff" point $r_0>0$, a point chosen to be as close as possible to the singular point $r=0$ where the boundary conditions are imposed and the actual numerical integration begins. As r_0 was allowed to approach zero, the values obtained by D02KDF were seen to approach the Padé values. In comparison, much less computational effort is involved in the Padé-CF approach. In addition, a measure of the accuracy of the perturbation method is provided by the upper and lower bounds yielded by successive convergents.

TABLE V. Rayleigh-Schrödinger perturbation coefficients $E^{(n)}$ for the KG π-mesonic atom with perturbed mass, i.e., $V(r)=-Z/r$ and $W(r)=\lambda r$. Here $K^2=L(L+1)$ and the unperturbed energy $E_0=E^{(0)}$ is given in Eq. (1.2).

n	$E^{(n)}$
0	E_0
1	$\dfrac{m^2Z^2-m^2K^2+2Z^2E_0^2+K^2E_0^2}{2Zm(m^2-E_0^2)}$
2	$-\dfrac{E_0}{8m^2Z^2(m^2-E_0^2)^3}(6m^2Z^4E_0^2-3m^4K^4+3m^4Z^2+9m^4Z^4-m^2Z^2E_0^2+6m^2K^4E_0^2-6Z^2K^2E_0^4-8Z^4E_0^4-2Z^2E_0^4-3K^4E_0^4-6m^4Z^2K^2+12m^2Z^2K^2E_0^2)$

IV. CONCLUDING REMARKS

In this paper, relativistic hypervirial and Hellmann-Feynman theorems have been used to generate perturbation expansions for the energies of radially perturbed Klein-Gordon equations. As in the Dirac case, an analysis of the continued fraction representations of these series reveals Stieltjes behavior for the perturbing scalar case.

It would be straightforward to extend the HVHF perturbative method to treat KG particles in screened Coulombic-type potentials of the form

$$V(r)=-\frac{Ze^{-\lambda r}}{r}, \quad (4.1)$$

as has been done for the Dirac equation [10] and for the nonrelativistic case [24].

The conjectures about the large-order behavior and summability properties of the perturbation expansions for Dirac and Klein-Gordon equations are based on numerical evidence. It would now be extremely desirable to develop a theoretical treatment of the large-order behavior of perturbation theory for these problems, perhaps analogous to the Bender-Wu WKB analysis for nonrelativistic anharmonic oscillators [24,21].

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APPENDIX: KG EQUATION WITH ATTRACTIVE COULOMBIC SCALAR AND VECTOR POTENTIALS

We consider the three-dimensional Klein-Gordon equation having the form ($\hbar=c=1$)

TABLE VI. Upper and lower bounds to energies E of Klein-Gordon π-mesonic atom ($N_r = L = 0$) with perturbed mass, i.e., $V(r) = -Z/r$ and $W(r) = \lambda r$ in Eq. (3.7), for various values of Z and λ. Each entry is the convergent $w_{39}(\lambda)$ of the Stieltjes continued-fraction representation (equivalently, the [19,19] Padé approximant) of the RS perturbation series, and represents an upper bound. The lower bound $w_{40}(\lambda)$ ([19,20] Padé) is obtained by replacing the final k digits of each entry with the k digits in parentheses.

λ \ Z	0.5	0.4	0.3	0.2
0.0	0.707 106 781 186 54	0.894 427 190 999 91	0.948 683 298 050 51	0.978 906 312 930 70
0.01	0.716 815 172 269 24	0.918 077 922 706 81	0.983 411 945 0(49)	1.026 683 9(09)
0.05	0.751 435 153 778 99	0.991 505 0(49)	1.079 797(62)	1.145 795(48)
0.1	0.788 775 203 61(59)	1.063 490(84)	1.170(69)	1.263(34)
0.2	0.852 303 690(62)	1.179 1(88)	1.316(05)	1.47(34)
0.3	0.906 822 3(16)	1.275 5(37)	1.443(09)	1.68(41)

$$\left[\nabla^2 + \left[E + \frac{Z_v}{r}\right]^2 - \left[m - \frac{Z_s}{r}\right]^2\right]\psi(\mathbf{r}) = 0 , \quad \text{(A1)}$$

where Z_v and Z_s denote the coupling constants for the vector and scalar potentials, respectively. After a separation of variables, $\psi(\mathbf{r}) = r^{-1}R(r)Y(\theta,\phi)$, one obtains the radial equation

$$\left[-\frac{d^2}{dr^2} + \frac{L(L+1) - Z_v^2 + Z_s^2}{r^2} - \frac{2(Z_v E + Z_s m)}{r} + (m^2 - E^2)\right]R(r) = 0 . \quad \text{(A2)}$$

As in standard treatments of the vector-Coulombic problem [1], we set $\rho = \beta r$, where $\beta^2 = 4(m^2 - E^2)$ to obtain the modified radial equation

$$\left[-\frac{d^2}{d\rho^2} + \frac{\Lambda^2}{\rho^2} - \frac{\lambda}{\rho} + \frac{1}{4}\right]P(\rho) = 0 , \quad \text{(A3)}$$

where

$$\Lambda^2 \equiv L(L+1) - Z_v^2 + Z_s^2 , \quad \text{(A4a)}$$

$$\lambda \equiv 2\beta^{-1}(Z_v E + Z_s m) > 0 . \quad \text{(A4b)}$$

The solution to Eq. (A3) is given by

$$P(\rho) = \rho^{S+1} W(\rho) e^{-\rho/2} , \quad \text{(A5)}$$

where $W(\rho)$ is given by a confluent hypergeometric function,

$$W(\rho) = {}_1F_1(-\lambda + S + 1, 2S + 2, \rho) . \quad \text{(A6)}$$

The condition that $P(\rho) \to 0$ as $\rho \to \infty$ implies that the confluent hypergeometric function in Eq. (A6) be a polynomial, i.e., that

$$\lambda - S - 1 = N_r = 0, 1, 2, \ldots . \quad \text{(A7)}$$

From the relation $S(S+1) = \Lambda^2$, we choose the positive root

$$S = -\tfrac{1}{2} + [(L + \tfrac{1}{2})^2 - Z_v^2 + Z_s^2]^{1/2} . \quad \text{(A8)}$$

From Eq. (A4b), we obtain the energy E of this system,

$$E = \frac{-Z_v Z_s + [Z_v^2 Z_s^2 - m^2(Z_s^2 - \lambda^2)(Z_v^2 + \lambda^2)]^{1/2}}{Z_v^2 + \lambda^2} , \quad \text{(A9)}$$

where $\lambda = N_r + S + 1$.

The HV recursion relations for this problem are

$$(k+1)[E^2 - m^2]\langle r^k\rangle = k[L(L+1) - Z_v^2 + Z_s^2 - \tfrac{1}{4}(k^2 - 1)]\langle r^{k-2}\rangle - (2k+1)(Z_v E + Z_s m)\langle r^{k-1}\rangle , \quad \text{(A10)}$$

which may be compared to the vector Coulomb case, Eq. (2.5). Radial scalar and/or vector perturbations of this system may now be studied in a manner analogous to that reported in Sec. III.

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