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Hydrogenic atoms in the external potential $V(r) = gr + \lambda r^2$: exact solutions and ground-state eigenvalue bounds using moment methods

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Abstract. An infinite number of exact solutions for the ground and excited states of an s-wave hydrogenic atom with the perturbation $V(r) = gr + \lambda r^2$ are constructed, subject to special relations between g, λ and the nuclear charge Z. A powerful method of Stieltjes moments is employed to generate rapidly converging upper and lower bounds to the ground-state energy $E_0(Z, g, \lambda)$ for arbitrary g, Z and positive λ. The accuracies of these bounds are relatively insensitive to the strength of the perturbation. The moment method also generates the exact s-wave ground-state solutions mentioned above.

1. Introduction

Radial hydrogenic perturbation problems with Hamiltonians of the general form (in atomic units)

$$\hat{H} = \tfrac{1}{2}\hat{p}^2 - Z/r + V(\boldsymbol{\beta}, r) \tag{1.1}$$

where $\boldsymbol{\beta}$ denotes a vector of coupling constants, have been studied in a wide variety of contexts. Special radial perturbations represent simplified versions of important physical situations encountered in atomic and molecular physics as well as astrophysics and solid state physics. For example, in the general family of perturbations $V = \beta r^p$, the case $p = 1$ corresponds to a spherical Stark effect in hydrogen (Austin 1981, Vrscay 1985) while $p = 2$ may be considered a spherical quadratic Zeeman effect (Killingbeck 1977, Avron 1981). Such potentials have also been studied in the context of non-relativistic quark confinement potentials in quantum chromodynamics (Eichten *et al* 1978, Quigg and Rosner 1979, Vrscay 1984). More complicated series expansions of the perturbation, such as

$$V(\beta, r) = \sum_{k=1} a_k (\beta r)^k \tag{1.2}$$

serve as important models of screened Coulomb potentials (Lai 1981).

The perturbation in (1.1) corresponding to $Z = 1$ and

$$V = 2\beta r + 2\beta^2 r^2 \qquad \beta \in \mathbb{R} \tag{1.3}$$

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has received much attention which, in fact, motivated this particular study. Killingbeck (1978b) discovered that a Rayleigh-Schrödinger perturbation series expansion for the ground-state energy, having the form

$$E(\beta) = -\tfrac{1}{2} + \sum_{n=1}^{\infty} E^{(n)}\beta^n \tag{1.4}$$

truncates after the first-order term. The underlying reason is that this particular Hamiltonian admits the exact ground-state solution $\psi(r) = \exp(-r - \beta r^2)$ with energy eigenvalue $E = -\frac{1}{2} + 3\beta$. The solution (and eigenvalue) are valid only for $\beta \geq 0$, corresponding to the region of quadratic integrability of the wavefunction. Saxena and Varma (1982a) formulated a perturbation theory for the region $\beta < 0$ in powers of $(-\beta)^{-1/2}$. They also constructed sets of exact s-wave polynomial solutions for both cases $\beta \geq 0$ and $\beta < 0$ (Saxena and Varma 1982b).

In this paper, we examine a generalisation of the potential in (1.3), namely the Hamiltonian

$$\hat{H} = \tfrac{1}{2}\hat{p}^2 - Z/r + gr + \lambda r^2 \tag{1.5}$$

where Z represents the variable (positive) nuclear charge and g and λ represent independent coupling constants, with the sole constraint that $\lambda > 0$. Our study serves two purposes.

(i) Using traditional methods we construct an infinite family of exact s-wave polynomial eigenfunctions of (1.5), subject to special relations between Z, g and λ. In the case $Z = 1$, $g = 2\beta$ and $\lambda = 2\beta^2$, these solutions reduce to those obtained by Saxena and Varma (1982b).

(ii) We employ a powerful method of moments (Handy and Bessis 1985) to generate upper and lower bounds which converge rapidly to the ground-state energy $E_0(g, \lambda)$. In addition, the moment method will also be shown to generate the exact s-wave solutions discussed above, again provided that the special relations between Z, g and λ exist.

2. Exact solutions

The Schrödinger differential eigenvalue equation for the s-wave Hamiltonian in (1.5) will be written as

$$\left(-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} - \frac{2Z}{r} + 2gr + 2\lambda r^2 - 2E\right)\psi(r) = 0. \tag{2.1}$$

We now assume power series solutions of the form

$$\psi(r) = \phi(r)\exp(-ar^2 - br) \tag{2.2}$$

where

$$\phi(r) = \sum_{m=0}^{\infty} c_m r^m. \tag{2.3}$$

Substitution into (2.1) yields

$$a = \left(\frac{\lambda}{2}\right)^{1/2} \qquad b = \frac{g}{(2\lambda)^{1/2}} \tag{2.4}$$

and the following three-term recurrence relations between the power series coefficients:

$$(m+2)(m+3)c_{m+2}+[2Z-2b(m+2)]c_{m+1}$$
$$+2[E+\tfrac{1}{2}b^2-a(2m+3)]c_m=0 \qquad m=0,1,2,\ldots. \tag{2.5}$$

For polynomial solutions $\phi(r)=\phi_n(r)$, where

$$\phi_n(r)=\sum_{m=0}^{n} c_m r^m \qquad n=0,1,2,\ldots \tag{2.6}$$

the recurrence relation (2.5) terminates if $c_{n+1}=0$ and $E+\frac{1}{2}b^2-a(2n+3)=0$, i.e.

$$E=\bar{E}_n\equiv(2n+3)\left(\frac{\lambda}{2}\right)^{1/2}-g^2/4\lambda. \tag{2.7}$$

The equations in (2.5) form a system of n linear homogeneous equations for the c_m, for which solutions are guaranteed provided the following determinantal condition is satisfied (Cramer's rule):

$$D_n(Z,g,\lambda)=\begin{vmatrix} Z-b & 1 & & & \\ 2na & Z-2b & 3 & & 0 \\ & 2(n-1)a & Z-3b & 6 & \\ & & \ddots & \ddots & \\ & 0 & & & \tfrac{1}{2}n(n+1) \\ & & & 2a & Z-(n+1)b \end{vmatrix}=0. \tag{2.8}$$

This condition provides a necessary relation between Z, g and λ to exist for each solution ψ_n with eigenvalue $\bar{E}_n$. An expansion about the last row or column of the determinant D_n in (2.8) gives a three-term recurrence relation for contiguous determinants, namely

$$D_i=[Z-(i+1)b]D_{i-1}-ai(i+1)D_{i-2} \qquad i=0,1,2,\ldots \qquad D_{-2}=0,\ D_{-1}=1. \tag{2.9}$$

Let us now mention that the special case of (2.1) studied by Saxena and Varma (1982b) corresponds to $Z=1$, $g=2\beta$ and $\lambda=2\beta^2$. The parameters in (2.4) become $a=\beta$ and $b=1$. The energies $\bar{E}_n$ of the exact s-wave polynomial solutions in (2.7) as well as the determinants D_n in (2.8) reduce to the two sets of results presented in the above-mentioned reference, dependent upon whether the parameter β is positive or negative.

3. Upper and lower bounds and exact solutions via moment methods

In this section, we employ a powerful moment method developed by Handy and Bessis (1985) which is based on the positivity property of the ground-state wavefunction. Its application to a number of problems has been outlined in the above reference. The power of the method is demonstrated in several properties. Its applicability is not restricted to special classes of potentials (e.g. bounded or positive definite); rather, it can accommodate general rational function potentials. Not being based on any conventional perturbative or variational method, it yields rapidly converging upper and lower

bounds for a wide range of coupling constant values (i.e. low field as well as high field). The moment method does not depend upon any form of basis function expansion. As such, its application to hydrogenic perturbation problems is not plagued by the existence of unperturbed continuum states.

It must be mentioned that other excellent methods of calculating ground- and excited-state eigenvalues have been derived for such one-dimensional systems; for example, the moment method of Killingbeck (1978a), cited by Richardson and Blankenbecler (1979) and Blankenbecler *et al* (1980), and simplified by Killingbeck *et al* (1985). An important feature of the present method is that this moment formulation simultaneously provides *upper* and *lower* bounds to eigenvalues. In usual practice, of course, widely separate techniques of calculating these bounds are employed, e.g. variational methods as opposed to intermediate Hamiltonian or inner projection methods. Our main goal here is to demonstrate how precise and rapidly converging upper and lower bounds may be obtained. Some surprises, even in one-dimensional cases, can occur. For example, a combined Padé Hellman-Feynman hypervirial approach yields a ground-state eigenvalue of $E_g = 1.017\,281\,60$ for the 'laser physics problem' ($\lambda = 0.1$, $g = 2$) of Lai and Lin (1982) while Hankel-Hadamard determinantal inequalities yield the exact bounds $1.017\,176 < E_g < 1.017\,185$ (Handy and Bessis 1985).

In our application of the moment method to the ground state of the Hamiltonian in (1.5), we first define

$$F(r) = r\exp(-ar^2 - br)\psi(r) \tag{3.1}$$

where $\psi(r)$ is the ground-state solution of the eigenvalue equation (2.1) and a and b are parameters given in (2.4). If we substitute $\psi(r)$ in (3.1) into (2.1), the following differential equation for $F(r)$ is obtained:

$$r\frac{d^2F}{dr^2} + 2(2ar^2 + br)\frac{dF}{dr} + [(b^2 + 2a + 2E)r + 2Z]F = 0. \tag{3.2}$$

Now introduce the moments of $F(r)$,

$$\mu_n = \int_0^\infty r^n F(r)\,dr \qquad n = 0, 1, 2, \ldots \tag{3.3}$$

which define a Stieltjes moment problem (Henrici 1977, Baker and Graves-Morris 1980) since $F(r) > 0$ for $r \in [0, \infty)$. If we multiply (3.2) by r^n and integrate over $[0, \infty)$, we obtain the following three-term recurrence relations for the moments μ_n:

$$\mu_{n+1} = \frac{[Z - (n+1)b]\mu_n + \frac{1}{2}n(n+1)\mu_{n-1}}{(2n+3)a - \frac{1}{2}b^2 - E}. \tag{3.4}$$

If we consider $F(r)$ to be normalised so that $\mu_0 = 1$, the moments μ_1 and μ_2 are then given by

$$\mu_1 = \frac{Z - b}{3a - \frac{1}{2}b^2 - E} \tag{3.5a}$$

$$\mu_2 = \frac{(Z - 2b)(Z - b) + 3a - \frac{1}{2}b^2 - E}{(5a - \frac{1}{2}b^2 - E)(3a - \frac{1}{2}b^2 - E)}. \tag{3.5b}$$

In general, we have

$$\mu_n = \frac{P_n(Z, g, \lambda, E)}{\prod_{k=0}^{n-1}[(2k+3)a - \frac{1}{2}b^2 - E]} \qquad n = 1, 2, 3, \ldots \tag{3.6}$$

where the polynomials P_i satisfy the recurrence relation

$$P_{i+1} = [Z - (i+1)b]P_i + \tfrac{1}{2}i(i+1)[(2i+1)a - \tfrac{1}{2}b^2 - E]P_{i-1}$$
$$P_0 = 1 \qquad P_1 = Z - b. \tag{3.7}$$

We now use the fact that a necessary and sufficient condition for the sequence of positive numbers μ_n to be moments of a non-negative function is that the Hankel-Hadamard determinants (Baker and Graves-Morris 1980), defined as follows:

$$H(n, m) = \begin{vmatrix} \mu_n & \mu_{n+1} & \cdots & \mu_{n+m} \\ \mu_{n+1} & \mu_{n+2} & \cdots & \mu_{n+m+1} \\ \vdots & \vdots & & \vdots \\ \mu_{n+m} & \mu_{n+m+1} & \cdots & \mu_{n+2m} \end{vmatrix} \tag{3.8}$$

satisfy the inequalities

$$H(0, m) > 0 \qquad \text{and} \qquad H(1, m) > 0 \qquad \text{for } m = 0, 1, 2, \ldots. \tag{3.9}$$

By increasing m in (3.9), i.e. by incorporating more moments $\mu_i(E)$ into the determinantal inequalities, stronger constraints on the energy E are being imposed in the form of upper and lower bounds. Let H_k, $k = 0, 1, 2, \ldots$, enumerate the alternating sequence of determinants $H(0,0)$, $H(1,0)$, $H(0,1)$, $H(1,1), \ldots$, i.e. $H_k = H(k \bmod 2, [k/2])$. (The case $H_0 = H(0,0) = \mu_0 = 1$ is trivial.) The moment of highest order occurring in H_k is μ_k. It is observed that the conditions $H_k > 0$, $k = 1, 2, 3, \ldots$, produce improvements in the upper and lower bounds to E_0, one at a time, in an alternating fashion. In the limit $k \to \infty$, all inequalities are satisfied only by E_0, the true ground-state eigenvalue of (2.1). The uniqueness of the distribution function $F(r)$, and hence the eigenfunction $\psi(r)$, may be argued on physical grounds where the ground state is non-degenerate. In addition, a sufficient (but not necessary) condition that the μ_i be moments of a unique distribution is given by Carleman's condition (Henrici 1977) that

$$\sum_{i=0}^{\infty} \mu_i^{-1/2n} = \infty. \tag{3.10}$$

This implies that the moments grow asymptotically at most as $\mu_n \sim (2n)!$, $n \to \infty$. In general, $\psi(r) \sim \exp(-ar^k)$ where $k \geq 1$, so that the μ_n grow at most like $n!$. This ensures that the determinantal inequalities $H_k > 0$ will select a unique ground-state energy E_0 as k increases to infinity.

Concerning the perturbation problem studied here, the first set of eigenvalue bounds come from the condition $H_1 = H(1,0) = \mu_1 > 0$. From (3.5*a*), there are three possibilities:

(i) case 1: $Z < b \Rightarrow E > 3a - \tfrac{1}{2}b^2$

(ii) case 2: $Z > b \Rightarrow E < 3a - \tfrac{1}{2}b^2$ (3.11)

(iii) case 3: $Z = b \Rightarrow E = 3a - \tfrac{1}{2}b^2$.

The latter equality in case 3 arises from the fact that the moments μ_i are necessarily positive and finite, by (3.3) and the existence of a ground-state eigenfunction. In this case, μ_1 assumes the indeterminate form 0/0. In fact, from (3.6), it follows that the condition

$$P_n(Z, g, \lambda, E)|_{E = \bar{E}_{n-1}} = 0 \qquad n = 1, 2, 3, \ldots \tag{3.12}$$

where the $\bar{E}_n$ are defined in (2.7), ensures that μ_n be positive and finite in the special case $E = \bar{E}_{n-1}$. Here we see that the moment equations generate the exact polynomial energies $\bar{E}_n$ obtained earlier. Indeed, from (2.9) and (3.7),

$$P_{n+1}(Z, g, \lambda, E)|_{E=\bar{E}_n} = D_n(Z, g, \lambda) \qquad n = 0, 1, 2, \ldots . \tag{3.13}$$

In other words, Cramer's rule in (2.8) for the existence of the polynomial solutions ϕ_n corresponds to the necessary indeterminacy relation $\mu_n = 0/0$ in (3.6).

The development of further bounds to E in closed form is tedious and we shall resort to numerical methods to extract accurate ground-state energies for several sets of parameters in the next section.

Recall that the methods of § 2 generated an infinite family of solutions $\psi_n(r) = \phi_n \exp(-ar^2 - br)$ with eigenvalues $\bar{E}_n$ as given by (2.7). Although $\psi_0(r)$ is clearly always a ground state, the number of nodes of ψ_n for $n > 1$ will be dependent upon the parameters Z, g and λ. All exact solutions ψ_n generated by the moment method, however, must be nodeless ground states, by virtue of (3.1). Consider, for example, the eigenstate ψ_1, given by (cf (2.5))

$$\psi_1(r) = c_0\left(1 - \frac{1}{Z-b}r\right)\exp(-ar^2 - br) \tag{3.14}$$

with eigenvalue $\bar{E}_1 = 5a - \frac{1}{2}b^2$. Note that $\psi_1(r)$ may or may not be a ground state, depending upon whether $Z < b$ or $Z > b$. (The case $Z = b$ corresponds to $D_0(Z, g, \lambda) = 0$ in (2.8), yielding $\psi_0(r)$.) The determinantal condition $D_1(Z, g, \lambda) = 0$ is

$$Z^2 - 3bZ + 2(b^2 - a) = 0 \tag{3.15}$$

which, when regarded as a quadratic equation in Z, has roots

$$Z_\pm = \tfrac{3}{2}b \pm \tfrac{1}{2}(b^2 + 8a)^{1/2}. \tag{3.16}$$

The moment condition $\mu_1 > 0$ must also be satisfied, however. From (3.5a), in which $E = \bar{E}_1$, it follows that $Z < b$. Since $Z_+ > 2b$ and $Z_- < b$, it follows that Z_- is the only admissible root of (3.16). Thus, $\psi_1(r)$ in (3.14) is nodeless for $Z = Z_-$.

We expect that this situation extends to each higher exact solution $\psi_n(r)$, i.e. at most one root Z_i of a higher degree polynomial corresponding to (3.15) would be admissible after all positivity conditions are imposed, yielding a nodeless ground state with energy $\bar{E}_n$.

We mention that the moment method is applicable to excited states in a natural way. To illustrate this briefly, consider the first excited state $\psi_1(r)$ as the *unique* square-integrable solution of the Schrödinger equation (2.1) with eigenvalue E_1 and having *exactly* one node. We may write

$$\psi_1(r) = (r - r_1)\bar{\psi}_1(r) \tag{3.17}$$

where $r_1 > 0$ and $\bar{\psi}_1(r)$ is a non-negative square-integrable function. Let $F(r)$ and $\bar{F}(r)$ be associated with $\psi_1(r)$ and $\bar{\psi}_1(r)$ as in (3.1). Now define the moments μ_n and $\bar{\mu}_n$ of $F(r)$ and $\bar{F}(r)$, respectively, as in (3.3). It follows that

$$\mu_n = \bar{\mu}_{n+1} - r_1\bar{\mu}_{n+1}. \tag{3.18}$$

The $\bar{\mu}_n$, which clearly define a Stieltjes moment problem, may be expressed in terms of the μ_n which are, in turn, functions of the unknowns E_1 and r_1. The Hankel–Hadamard inequalities for the $\bar{\mu}_n$ will now impose constraints on E_1 and r_1 in the form of converging upper and lower bounds on each parameter. It is interesting that

this moment approach locates precisely not only the energy eigenvalue but the position of the node of the eigenstate, suggesting a deeper physical connection. A detailed study of excited states for this problem is, however, beyond the scope of the present paper.

4. Numerical results

Before beginning this section, we mention that a coordinate scaling argument yields the following relationship between the parameters Z, g, λ and E:

$$E(Z, g, \lambda) = Z^2 E\left(1, \frac{g}{Z^3}, \frac{\lambda}{Z^4}\right). \tag{4.1}$$

We have not made use of this relationship in the present study. However, one may verify that the upper and lower bounds obtained by the Hankel-Hadamard inequalities fulfil this relationship exactly. This explains, in part, the independence of the relative errors in bounds with respect to coupling constant values.

The algorithm employed in this study begins with the bounds in (3.11) and searches the real-E line for nested intervals of positivity of the higher-order Hankel determinants H_k, $k \geq 2$. The endpoints of these intervals correspond to increasingly accurate upper and lower bounds to E. As k increases, the condition $H_k > 0$ generally improves the bounds in an alternating fashion.

We mention that the Hankel determinants $H(n, m)$ may be easily and rapidly calculated via Jacobi's identity (Henrici 1974):

$$[H(n, m)]^2 - H(n-1, m)H(n+1, m) + H(n-1, m+1)H(n+1, m-1) = 0. \tag{4.2}$$

If the determinants $H(n, m)$, $n \geq 0$, are arranged in a triangular array as shown in figure 1, they are linked together by (4.2) in a star-like pattern. The first two columns of the table ($m = -1, 0$) are easily initialised and (4.2) may be rearranged to calculate columns corresponding to $m = 1, 2, 3, \ldots$, recursively. From (3.8) and (3.9), we need consider only the two tables corresponding to $n = 0$ and 1. To determine eigenvalue bounds for given set of coupling constants, the trial values of E are used to calculate the moments in the second column of the table via (3.6). The Hankel array of figure 1 is calculated outward to the desired determinant H_k, which is then checked for positivity.

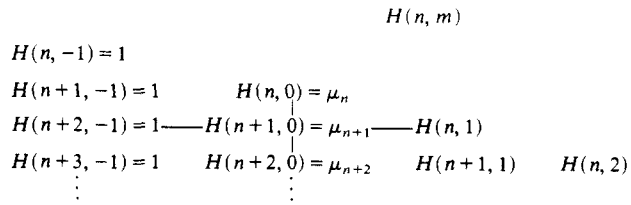

Figure 1. The lower triangular array of Hankel determinants $H(n, m)$. Five elements connected by Jacobi's identity in (4.2) are shown to form a four-pointed star. Equation (4.2) may be rearranged to calculate columns of this array from left to right. From (3.9), the values of n relevant to the moment method are $n = 0$ and 1.

A note of caution concerning the Jacobi method of (4.2) must be made here. For some values of the parameters of this problem, it is possible that neighbouring entries in the Jacobi table become so close in value, relative to the fixed precision used, that the algorithm becomes plagued with a 'small denominator problem' causing either inaccurate bound estimates or computer exponent overflows. When this occurs, one may circumvent such problems by evaluating the Hankel determinants $H(m, n)$ directly by using a library subroutine. Of course, such direct calculations are performed at the expense of computer time.

In order to illustrate the rapid rate of convergence afforded by the moment method, we introduce the errors

$$d_k^{(\pm)} = |E_k^{(\pm)} - E_0| \tag{4.3}$$

where $E_k^{(+)}$ and $E_k^{(-)}$ denote, respectively, the upper and lower bounds to the true ground-state energy E_0 obtained from the condition $H_k > 0$, which employs the moments $\mu_0 \ldots \mu_k$. Table 1 presents errors for three sets of parameter values $Z = 1$, $g = \lambda = 0.1$, 1 and 5. An exponential rate of convergence to E_0 is observed in all cases. We also note that, for a given value of k, the accuracies in the bounds are similar over the range of coupling constant values; in fact, the accuracy is seen to improve with increasing strength of the perturbation.

Table 1. Deviations from the exact ground-state energies for the three sets of parameter values $(Z, g, \lambda) = (1, 0.1, 0.1)$, $(1, 1, 1)$, $(1, 5, 5)$. The notation 3.6 (−3) denotes 3.6×10^{-3}. The index k denotes the maximum number of moments used in the calculation of the bounds. The final entries in each column denote the inequalities established from the case $k = 12$.

k	$Z = 1$	$g = \lambda = 0.1$	$Z = 1$	$g = \lambda = 1$	$Z = 1$	$g = \lambda = 5$
6	2.2 (−2)	3.6 (−3)	1.9 (−3)	2.7 (−4)	6.0 (−5)	5.0 (−4)
7	1.7 (−3)	3.6 (−3)	9.5 (−5)	2.7 (−4)	6.0 (−5)	1.7 (−5)
8	1.7 (−3)	3.1 (−4)	9.5 (−5)	1.5 (−5)	2.3 (−6)	1.7 (−5)
9	1.2 (−4)	3.1 (−4)	5.1 (−6)	1.5 (−5)	2.3 (−6)	6.3 (−7)
10	1.2 (−4)	2.4 (−5)	5.1 (−6)	8.8 (−7)	1.0 (−7)	6.3 (−7)
11	8.9 (−6)	2.4 (−5)	2.7 (−7)	8.8 (−7)	1.0 (−7)	2.5 (−8)
12	8.9 (−6)	1.8 (−6)	2.7 (−7)	5.2 (−8)		2.5 (−8)
12	$-0.185\,012 < E_g < -0.185\,001$		$1.332\,8452 < E_g < 1.332\,8455$		$5.157\,751\,48 < E_g < 5.157\,751\,51$	

Tables 2, 3 and 4 list bounds for $E(Z, g, \lambda)$ in cases where two of the three parameters, Z, g and λ, are fixed and the third is varied. In table 2, all entries were calculated using the moments $\mu_0, \mu_1, \ldots, \mu_{15}$, corresponding to the condition $H_{15} = H(1, 7) > 0$. In table 3, the subscript N of the highest moment μ_N employed to achieve the accuracy of each entry is shown. With regards to the entries in table 4, we mention that the case $Z = 0$, $g = 0$ and $\lambda = 1$ corresponds to a three-dimensional harmonic oscillator

$$\hat{H} = \tfrac{1}{2}\hat{p}^2 + r^2 \tag{4.4}$$

with ground-state eigenvalue $E_0 = 3/\sqrt{2}$. The moment method yields this exact result

Table 2. Lower and upper bounds, $E^{(-)}$ and $E^{(+)}$, respectively, to the ground-state energy $E(Z, g, \lambda)$ for $Z=1$ and $g=0$ and λ variable. The moments μ_0 to μ_{15} were employed.

	$Z=1, g=0$	
λ	$E^{(-)}(Z, g, \lambda)$	$E^{(+)}(Z, g, \lambda)$
0.1	−0.296 088	−0.296 087
0.5	0.179 6683	0.179 6690
1.0	0.593 7711	0.593 7716
2.0	1.223 7050	1.223 7054
5.0	2.561 7326	2.561 7330
10.0	4.150 1236	4.150 1239
20.0	6.479 9505	6.479 9508
50.0	11.265 4474	11.265 4477
100.0	16.805 2478	16.805 2481
1000.0	59.375 4689	59.375 4694
2000.0	85.734 8038	85.734 8042
5000.0	138.557 1975	138.557 1981

Table 3. Lower and upper bounds to the ground-state energy $E(Z, g, \lambda)$ for $Z=1$, $\lambda=1$, g variable. The entries in the final column denote the subscript N of the highest-order moment μ_N employed for each g value.

	$Z=1, \lambda=1$		
g	$E^{(-)}(Z, g, \lambda)$	$E^{(+)}(Z, g, \lambda)$	N
−2.0	−1.171 673 5848	−1.171 673 5845	29
−1.0	−0.226 186 8754	−0.226 186 8749	25
−0.5	0.196 002 3855	0.196 002 3858	23
−0.1	0.515 935 2547	0.515 935 2552	21
0.0	0.593 771 2791	0.593 771 2799	31
0.1	0.670 814 0275	0.670 814 0280	31
0.5	0.971 615 6507	0.971 615 6513	29
1.0	1.332 845 4922	1.332 845 4923	19
2.0	2.014 906 2264	2.014 906 2265	15
3.0	2.654 098 5688	2.654 098 5689	11
5.0	3.837 429 8775	3.837 429 8776	11

as case 3 of (3.11), since $Z=b=0$ and $a=1/\sqrt{2}$ (cf (2.4)). One can note, in fact, that this table is but a variation of table 2, by virtue of the scaling relation in (2.10).

5. Summary

A powerful method of moments has been employed to generate rapidly converging upper and lower bounds to the ground-state energy of a radially perturbed hydrogenic atom. Accurate values of the energy are obtained over a wide spectrum of coupling constant values. The method is applicable to general quantum mechanical Hamiltonians with rational function potentials. In addition, the positivity criterion of the moments generates an infinite family of exact s-wave solutions subject to special relations existing between the coupling constants.

Table 4. Lower and upper bounds, $E^{(-)}$ and $E^{(+)}$, respectively, to the ground-state energy $E(Z, g, \lambda)$ for $g = 0$, $\lambda = 1$ and the nuclear charge Z variable. The moments μ_0 to μ_{15} were employed.

	$g = 0, \lambda = 1$	
Z	$E^{(-)}(Z, g, \lambda)$	$E^{(+)}(Z, g, \lambda)$
0.1	1.985 547 78	1.985 547 79
0.5	1.407 889 7	1.407 889 8
1.0	0.593 771 1	0.593 771 6
2.0	−1.443 047	−1.443 041
5.0	−12.382 1	−12.381 6
10.0	−49.97	−49.96
20.0	−200.01	−199.96

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References

Austin E J 1981 *Mol. Phys.* **40** 893
Avron J E 1981 *Ann. Phys., NY* **131** 73
Blankenbecler R, DeGrand T and Sugar R L 1980 *Phys. Rev.* D **21** 1055
Baker G A Jr and Graves-Morris P 1980 *Pade Approximants, Part I: Basic Theory, Part II: Extensions and Applications* (Reading, MA: Addison-Wesley)
Eichten E, Gottfried K, Kinoshita T, Lane K D and Yan T-M 1978 *Phys. Rev.* D **17** 3090
Handy C and Bessis D 1985 *Phys. Rev. Lett.* **55** 931
Henrici P 1974 *Applied and Computational Complex Analysis* vol 1 (New York: Wiley-Interscience)
—— 1977 *Applied and Computational Complex Analysis* vol 2 (New York: Wiley-Interscience)
Killingbeck J 1977 *Rep. Prog. Phys.* **40** 963
—— 1978a *Phys. Lett.* **63A** 223
—— 1978b *Phys. Lett.* **67A** 13
Killingbeck J, Jones M N and Thompson M J 1985 *J. Phys. A: Math. Gen.* **18** 793
Lai C S 1981 *Phys. Rev.* A **23** 455
Lai C S and Lin H E 1982 *J. Phys. A: Math. Gen.* **15** 1495
Quigg C and Rosner J L 1979 *Phys. Rep.* **56** 167
Richardson J L and Blankenbecler R 1979 *Phys. Rev.* D **19** 496
Saxena R P and Varma V S 1982a *J. Phys. A: Math. Gen.* **15** L149
—— 1982b *J. Phys. A: Math. Gen.* **15** L221
Vrscay E R 1984 *Phys. Rev. Lett.* **53** 2521
—— 1985 *Phys. Rev.* A **31** 2054