ERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, VOL. XXXVI, 61–65 (1989)

On the Ricatti Equation for Eigenvalue Problems

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Abstract

The Riccati equation is shown to be suitable for obtaining implicit approximate analytic expressions for eigenvalues of quantum-mechanical systems. The Hamiltonian operator $H = (1/2)p^2 - (Z/r) + \lambda r^2$ ısed as a test example, and the resulting formulae are modified to deal with the Zeeman effect in hydrogen.

The Riccati equation proves to be useful in large-order perturbation calculations cause it leads to closed quadrature expressions for the coefficients of the perturba-ın series (Ref. 1 and references therein). A nonperturbative approach based on the nilarity transformation proposed by Hall [2] was shown to improve the perturbation pansion considerably [3, 4] (an interesting alternative method was discussed by llingbeck [5]). A similar procedure, although with an ansatz properly adapted to und systems, was tried by Fernández and Castro [6].

In this letter we investigate some properties of the approximate eigenvalues ob-ned from Hall's method [2–4]. To this end the Hamiltonian operator

$$H = -\frac{1}{2}\Delta + V, \qquad V = -\frac{Z}{r} + \lambda r^2 \tag{1}$$

most suitable because its eigenvalues $E(Z, \lambda)$ and eigenfunctions are exactly known ıen either $Z = 0$ or $\lambda = 0$.

The perturbation series

$$E(Z, \lambda) = \sum_{j=0}^{\infty} E_j \lambda^j, \tag{2}$$

known to be asymptotic divergent [7], and the coefficients E_i are easily calculated om the Riccati equation [1] or through the hypervirial perturbative method [8]. It llows from the scaling law $E(Z, \lambda) = \lambda^{1/2} E(Z\lambda^{-1/4}, 1)$ that $E(Z, \lambda)$ has the covergent pansion [7]

$$E(Z, \lambda) = \lambda^{1/2} \sum_{j=0}^{\infty} e_j \lambda^{-j/4}. \tag{3}$$

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Therefore, an acceptable approximation to $E(Z, \lambda)$ has to obey (2) and (3) as accurately as possible.

The radial part of the Schrödinger equation (for the sake of simplicity we only consider the ground state)

$$\left(-\frac{1}{2}D^2 - \frac{1}{r}D + V - E\right)\Phi = 0, \qquad D = \frac{d}{dr}, \tag{4}$$

can be rewritten as a Riccati equation for $f = -\Phi'/\Phi$:

$$f' - f^2 + \frac{2}{r}f + 2(V - E) = 0. \tag{5}$$

This last equation can easily be shown to be equivalent to that obtained through Hall's method [4] by introducing $f(r) = Z - S(r)$. Because $f(r)$ is a regular function, we seek a solution of Eq. (5) of the form

$$f(r) = \sum_{n=0}^{\infty} f_n r^n. \tag{6}$$

The coefficients f_n are found to obey

$$f_n = \frac{1}{n+2}\left[\sum_{j=0}^{n-1} f_j f_{n-j-1} + 2Z\,\delta_{n0} + 2W\,\delta_{n1} - 2\lambda\,\delta_{n3}\right], \tag{7}$$

in which W stands for the approximate eigenvalue.

We first consider the trivial case $Z = 0$. A straightforward calculation shows that $f_{2k} = 0$ $(k = 0, 1, \ldots)$ for all W values and that $F_1 = (2\lambda)^{1/2}$ and $f_{2k+3} = 0$ provided $W = 3/2\,(2\lambda)^{1/2}$. The exact ground-state wave function and energy are thus obtained.

When $Z\lambda \neq 0$ the exact solution cannot be found, but the result above suggests that there may be a root of $f_n = 0$ $(n > 1)$ which is an acceptable approximation to E. Without loss of generality we consider $Z = 1$. The coefficients f_n prove to be polynomial functions of W and λ, and we have analytically calculated them for all $n \leq 16$ by means of the algebraic processor REDUCE. For example, from $f_n = 0$, $n = 3, 4, 5$, and 6 we obtain

$$w^2 + 3w - 18\lambda = 0, \tag{8a}$$

$$w^2 + \frac{6}{7}w - \frac{36}{7}\lambda = 0, \tag{8b}$$

$$w^3 + \frac{67}{8}w^2 + 3w - 18w\lambda - 18\lambda = 0, \tag{8c}$$

$$w^3 + \frac{411}{164}w^2 + \frac{18}{41}w - \frac{423}{41}w\lambda - \frac{108}{41}\lambda = 0, \tag{8d}$$

respectively, where $w = 2W + 1$. It can easily be shown that W can be expanded

$$W = \lambda^{1/2}\sum_{j=0}^{\infty} w_j \lambda^{-j/2}, \tag{9b}$$

\ = 0 and $1/\lambda = 0$, respectively. These equations do not exactly agree with the ones, Eqs. (2), (3). For instance, the proper roots of $f_{2k+1} = 0$ and $f_{2k+2} = 0$), 1, ...) will satisfy $W_j = E_j$ only for $j \le k$. This result is due to the fact that rturbation corrections to $f(r)$ are polynomials where the highest power of r ;es with the perturbation order. Since the Taylor series for W approaches the perturbation series (2) as k increases, one may believe that W will tend to E. vever, large-order numerical calculation shows that the procedure is divergent, gh quite accurate results are obtained for moderately large k values. This be- is reminiscent of the perturbation series, although results from the present pro- are by far more accurate. For every finite k value the asymptotic behavior of E_i ($i \to \infty$) will be quite different, as shown by the fact that the Taylor series has a finite convergence radius determined by a branch point $\lambda_b = \lambda(W_b)$, $\partial\lambda/\partial W$ $(W = W_b) = 0$.

then calculate the limit

$$L = \lim_{\lambda\to\infty} w^2/\lambda . \tag{10}$$

$_{2k+1} = 0$ $(k = 1, 2, \ldots)$ we obtain the exact answer $L = E(0,1)^2 = 18$. On the ıand, the values of W for $f_{2k+2} = 0$ yield the sequence in Table I which appears verge quickly from below toward the same value of L. We cannot at present ıt for this surprising behavior.

worth noting that the large λ expansions for E and W do not exactly agree, :he odd powers of $\lambda^{-1/4}$ do not appear in the latter. This result may be due to :t that the method does not distinguish between the actual potential (1) and $= -Z/x + \lambda x^2$ $(-\infty < x < \infty)$ for which the odd corrections vanish.*

formulae for the preceding simple model can be applied, with appropriate :s, to the much more interesting problem of the Zeeman effect in hydrogen

$$V = -\frac{1}{r} + \frac{1}{2}\beta^2(x^2 + y^2). \tag{11}$$

way we avoid working with a Riccati equation in two dimensions. We can d in two different ways. First we use the spherical model with the perturbation

TABLE I. Limit (10) for a root of $f_{2k+2} = 0$.

k	L	k	L
1	5.1429	5	16.4671
2	10.3171	6	17.1143
3	13.4895	7	17.4917
4	15.3638		

TABLE II. Ground-state energy for the hydrogen atom in a uniform magnetic field from Eqs. (8c) ($\lambda = \beta^2/3$) and (12) ($\lambda = \beta^2/2$).

β	E [Eq. (8c)]	E [Eq. (12)]	E_{exact} (Ref. 11)
0.1	−0.4903	−0.4902	−0.49038
0.5	−0.3240	−0.3132	−0.33117
1.0	−0.0070	0.0491	−0.02221
10.0	8.94	8.80	7.78462
20.0	20.85	18.79	17.199
50.0	57.39	48.78	46.211
100.0	118.6	98.77	95.273

$1/3\,\beta^2 r^2$ which approximately mimics the quadratic term in (11) for moderate values of λ [4, 8, 9]. Second, we rewrite Eq. (8c) as

$$w^3 + Aw^2 + B\lambda w + Cw + D\lambda = 0\,, \tag{12}$$

and set A, B, C, and D so that $W_1 = 2$, $W_2 = 53/3$, $W_3 = 5581/9$ (the actual Zeeman perturbation corrections for the ground-state energy [10]), and $(\lambda^{-1/2}W)\,(\lambda \to \infty) = 2$. We have $A = 3.68592$, $B = -8$, $C = 1.52687$, and $D = -6.10750$.

Table II shows that both procedures yield upper bounds to the energy [4, 8, 9] and that the former is more accurate for small values of λ, whereas the latter is preferable for large ones. This behavior is a consequence of the fact that we have fixed B, so that the exact strong-field limit is obtained.

The main advantage of the latter method is that we can in principle take into account as many perturbation corrections as desired by simply considering a large enough value of n. This effect cannot be so easily achieved through a simple change in the perturbation term [4, 8, 9]. Our method, however, becomes very tedious for larger perturbation orders, and a systematic treatment of the polynomials is at present being examined.

Acknowledgment

J. F. O. thanks the National Science Council of the Republic of China for support of a visiting professorship at National Tsing Hua University.

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d January 13, 1988
d for publication October 17, 1988