Large-Order Perturbation Theory in the Stark-Zeeman Effect for Parallel Fields

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For the ground-state hydrogen atom in parallel electric and magnetic fields the coefficients in the double perturbation series are calculated to large order and certain asymptotic recurrences are stated. With use of only the *real* coefficients, the *complex* energy eigenvalue is obtained as a function of both field strengths by rational approximant methods. This represents the first application of two-variable approximants to the calculation of eigenvalues for a physical system.

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Over the last several years, rapid progress has been made in summing strongly divergent perturbation series, in large part because of interest in renormalizable field theories. For the particular cases of the hydrogenic Stark and Zeeman problems,[1] the energy expansions are available to large order[2-7] and are summable by either Borel[8,9] or Padé[7,9-11] methods. We report the first extension of rational approximant techniques to the more complicated case of the hydrogen atom in parallel electric and magnetic fields, wherein summation of a double Taylor series is required. Numerical analytic continuation of the rationally summed perturbation series for the ground state is shown to yield a resonance position and width associated with Stark tunneling along the common field axis. Additionally, we state some empirical asymptotic recurrences between the perturbation coefficients (along the lines of Bender-Wu formulas[6,12,13]).

The wave function and energy were obtained order by order by transforming the inhomogeneous differential perturbation equations into difference equations. (The basic idea here is not new,[7,14] but several of the details are.) The Hamiltonian (in atomic units) for the electric field $\vec{F}$ and the magnetic field $\vec{\gamma}$ both in the z direction is

$$H = -\tfrac{1}{2}\nabla^2 + \tfrac{1}{2}\gamma L_z + \tfrac{1}{8}\gamma^2\rho^2 + Fz - r^{-1}, \tag{1}$$

where $\rho = (x^2+y^2)^{1/2}$. The value $\gamma = 1$ corresponds to a magnetic field of 2.35×10^9 G, and $F = 1$ to an electric field of 5.14×10^9 V/cm. The Hamiltonian, energy, and wave function may all be expanded in the powers $F^i(\gamma^2/8)^j$, and, on close examination, it becomes apparent that the structure of the resulting $\Psi^{(i,j)}$, including all contributions from the continuum automatically, can be written in definite form. Eventually, we find

$$\Psi^{(i,j)}(\vec{r}) = \pi^{-1/2}e^{-r}z^{\epsilon}S^{(i,j)}(r,\rho), \tag{2}$$

where $\epsilon = 0$ (1) for i even (odd), and $S^{(i,j)}$ is a finite polynomial in r and ρ^2:

$$S^{(i,j)}(r,\rho) = \sum_{k=0}^{M(i,j)} \rho^{2k} f_k^{(i,j)}(r), \tag{3}$$

$$f_k^{(i,j)}(r) = \sum_{l=0}^{N(i,j,k)} c_{k,l}^{(i,j)} r^l. \tag{4}$$

The limits in these sums are given by

$$M(i,j) = j + [\tfrac{1}{2}i], \tag{5}$$

$$N(i,j,k) = \begin{cases} 2M(i,j)+i-k, & 0 \le k \le j, \\ 2M(i,j)+i+j-2k, & j \le k \le M(i,j). \end{cases} \tag{6}$$

By inserting these results into the perturbation equation of order (i,j), a *linear* system of inhomogeneous equations is obtained between the energy and the set of $c_{k,l}^{(i,j)}$ for this order. This system of equations is not only triangular, but sparse as well, and so can be easily programmed.

The resulting energy expansion is of the form

$$E = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \epsilon^{(m,n)} F^{2m} (\gamma^2/8)^n. \tag{7}$$

We have calculated the $\epsilon^{(m,n)}$ out to $m,n = 10$ in single-precision arithmetic (retaining at worst about 11 significant figures out of 15 on a Cyber 720) and out to $m,n = 8$ in double precision. The results for $m,n \le 5$ (obtainable in principle as ratios of integers) are given in Table I. The numbers for $n = 0$ (pure Stark) and for $m = 0$ (pure Zeeman) have been checked with the known results.[2-7] Of the cross terms, $\epsilon^{(1,1)}$ and $\epsilon^{(1,2)}$ have been checked against the calculations of Lambin, Van Hay, and Kartheuser.[15] Note that $\epsilon^{(m,n)}$ has the consistent phase $(-)^{n+1}$, independent of m.

The ability to calculate the perturbation coefficients to high order for the single-field cases has kindled a strong interest in their asymptotic

TABLE I. The $\epsilon^{(m,n)}$, as defined by Eq. (7), for $m,n \geq 5$. The number in parentheses is the power of 10 by which the entry is multiplied.

m	n	$\epsilon^{(m,n)}$	m	n	$\epsilon^{(m,n)}$	m	n	$\epsilon^{(m,n)}$
0	0	−5.000 000 000 0000(−1)	2	0	−5.554 687 500 0000(+1)	4	0	−7.942 369 264 5264(+5)
0	1	2.000 000 000 0000	2	1	3.983 671 875 0000(+3)	4	1	1.910 936 574 4647(+8)
0	2	−1.766 666 666 6667(+1)	2	2	−4.178 190 390 6250(+5)	4	2	−4.696 729 842 5958(+10)
0	3	6.201 111 111 1111(+2)	2	3	5.860 781 407 5521(+7)	4	3	1.338 997 775 1365(+13)
0	4	−3.995 814 259 2593(+4)	2	4	−1.054 805 236 9070(+10)	4	4	−4.528 964 925 0725(+15)
0	5	3.862 135 590 4938(+6)	2	5	2.377 968 348 2567(+12)	4	5	1.817 103 747 2195(+18)
1	0	−2.250 000 000 0000	3	0	−4.907 771 484 3750(+3)	5	0	−1.945 319 604 6650(+8)
1	1	3.975 000 000 0000(+1)	3	1	7.191 631 699 2188(+5)	5	1	6.904 891 276 2458(+10)
1	2	−2.049 791 666 6667(+3)	3	2	−1.215 529 745 2050(+8)	5	2	−2.326 311 127 2397(+13)
1	3	1.717 834 027 7778(+5)	3	3	2.512 104 570 5320(+10)	5	3	8.773 893 799 2619(+15)
1	4	−2.025 806 539 5139(+7)	3	4	−6.350 659 614 9332(+12)	5	4	−3.838 879 188 1669(+18)
1	5	3.161 543 545 8644(+9)	3	5	1.947 690 453 6922(+15)	5	5	1.957 391 948 8509(+21)

natures (see, e.g., Ref. 9). From examination of the $\epsilon^{(m,n)}$ for $m \leq 2$, $n \leq 20$ and $m \leq 20$, $n \leq 2$, we conjecture the following asymptotic recurrences:

$$\epsilon^{(m,n)}/\epsilon^{(m-1,n)} \simeq (\tfrac{3}{2})^2 2m(2m+4n-1), \quad m \gg 0,\ n \simeq 0, \tag{8}$$

$$\epsilon^{(m,n)}/\epsilon^{(m,n-1)} \simeq -(8/\pi^2)2n(2n+6m), \quad n \gg 0,\ m \simeq 0. \tag{9}$$

As is easily verified, Eqs. (8) and (9) are consistent with the Bender-Wu formulas for the Stark[12] and Zeeman[6,13] problems, respectively. Further information along these lines should be obtainable if the coefficients can be calculated to higher order. A theoretical derivation of the precise asymptotic nature of the $\epsilon^{(m,n)}$ would prove more challenging.

Once the energy coefficients have been obtained, they can be used to form various generalizations of Padé approximants[16] (PA's) to two variables. The choice made here is the Chisholm approximant (CA),[17]

$$[m/m] = \Big(\sum_{\alpha=0}^{m}\sum_{\beta=0}^{m} a_{\alpha\beta}x^{\alpha}y^{\beta}\Big)\Big/\Big(\sum_{\mu=0}^{m}\sum_{\nu=0}^{m} b_{\mu\nu}x^{\mu}y^{\nu}\Big), \tag{10}$$

which has the felicitous property of reducing to the appropriate PA whenever one of the variables vanishes. Determination of the a's and b's requires all of the $\epsilon^{(i,j)}$ for $i,j \leq 2m$. Thus it was possible to form up to the [5/5] CA. The results of using the [4/4] and [5/5] CA's are compared for select values of F and γ in Table II, indicating that this is indeed a reliable way of summing the double asymptotic series. For strong enough fields, of course, the [5/5] CA also becomes ineffective. This can be gauged by the accurate results, also listed, for the pure Stark *positions* and Zeeman energies.

In the Zeeman limit, the resulting PA's are known to converge (although slowly[7]) to the correct bound-state eigenvalue. It was initially hoped that, in the Stark limit, the PA's for the real perturbation series would correspondingly converge to the resonance positions.[4,10] Reinhardt[11] has pointed out that one only gets quasi-convergence in this case because the poles and zeros of the (diagonal) PA's all lie along the real F axis, eventually spoiling the convergence. He further showed that there are at least two meth-

TABLE II. The CA's of Eq. (10) for different values of F and γ.

F	γ	Chisholm approximants [4/4]	[5/5]	Exact
0.0	0.2	−0.4904	−0.4904	−0.4904[a]
0.0	0.6	−0.4278	−0.4277	−0.4275[a]
0.0	1.0	−0.3392	−0.3367	−0.3312[a]
0.04	0.2	−0.4938	−0.4938	···
0.04	0.6	−0.4310	−0.4323	···
0.04	1.0	−0.3480	−0.3539	···
0.02	0.0	−0.5009	−0.5009	−0.5009[b]
0.06	0.0	−0.5084	−0.5099	−0.5092[b]
0.10	0.0	−0.5801	−0.5396	−0.5274[b]
0.02	0.4	−0.4654	−0.4653	···
0.06	0.4	−0.4711	−0.4718	···
0.10	0.4	−0.4828	−0.4712	···

[a] Galindo and Pasqual (Ref. 5).
[b] Benassi *et al.* (Ref. 12).

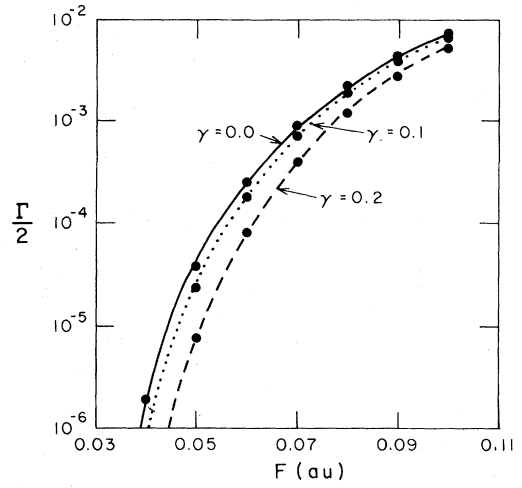

FIG. 1. Resonance width $\Gamma/2$ vs F for $\gamma=0.0$, 0.1, and 0.2. The dots are the accurate values obtained from the complex coordinate calculations which agree with Benassi and Greschi's results for $\gamma=0.0$.

ods which not only avoid this problem, but obtain the *complex* Stark eigenvalues using as input only the *real* perturbation coefficients. In one of the methods, the Stark PA's were evaluated at several points in the complex F plane (away from the zeros and poles), followed by numerical analytic continuation (via continued fractions[18]) back to the real axis. Although this procedure is not systematic, it performs reasonably well in obtaining the complex eigenvalue and may be carried over directly to the parallel-fields case by using CA's rather than PA's.[19] Results for the imaginary part of the energy obtained with the [5,5] CA are shown in Fig. 1. For comparison, we have also calculated accurate values by the complex coordinate method,[20] verifying the perturbation results. It is apparent from Fig. 1 that the effect of these sizable magnetic fields is to decrease the width of the resonance.

In order to avoid inadvertantly evaluating the approximants near singular points, we have examined the positions of the zeros and poles as either field is varied with the other fixed. Table III lists the [5,5] zeros and poles (in the variables F^2) for a value of γ used in Fig. 1. The strong overlappings of the small-F^2 values are increasingly disrupted as γ is increased, eventually leading to the appearance of complex zeros and poles. Similar results occur as a function of γ^2 for fixed F.

Thus it has been demonstrated that the complex energies for the hydrogen atom in parallel electric and magnetic fields can be evaluated by a combination of perturbation theory and rational approximant techniques. The current method for obtaining the $\epsilon^{(m,n)}$ could probably be coerced into yielding at least a few more orders of the energy for the same number of orders of the wave function by a generalization of Wigner's "$2n+1$ rule"[21] to double perturbation theory. Alternative approaches which may be more efficient are logarithmic perturbation theory (discussed briefly for the present problem by Turbiner[14]), or a generalization of the hypervirial-perturbation technique[4] to the double perturbation problem. Also, the SO(4,2) algebraic methods, which yield the same results as the procedure used here, may be more suitable in considering higher states.[7] The success of the current approach suggests that these generalizations may be tractable.

TABLE III. Location of the zeros and poles of the [5/5] CA as a function of F^2 for $\gamma = 0.2$. The number in parentheses is the power of 10 by which the entry is multiplied.

	Zeros	Poles
$F^2=$	1.190 0128(−3)	$F^2=$ 1.190 0128(−3)
	2.700 6377(−3)	2.700 6186(−3)
	6.874 7238(−3)	6.867 3071(−3)
	2.888 6628(−2)	2.770 3849(−2)
	−9.037 2871(−1)	6.602 2341(−1)

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