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Complex energies from real perturbation series for the LoSurdo-Stark effect in hydrogen by Borel-Padé approximants

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The resonance energies for the hydrogen atom in an electric field, both the real and imaginary parts, have been calculated together from the real Rayleigh-Schrödinger perturbation series by Borel summation. Padé approximants were used to evaluate the Borel transform. The numerical results compare well with values obtained by the complex-coordinate variational method and by sequential use of Padé approximants.

I. INTRODUCTION

There have been many calculations of the energy and ionization rate for the hydrogen atom in an electric field, the resonances of the LoSurdo-Stark effect.[1–25] Although it has been known for many years that the Rayleigh-Schrödinger perturbation theory (RSPT) for this system is Borel summable,[26] which is of utmost importance in the definition of the resonances from the divergent power series, nevertheless this fact has not been exploited computationally.[27] The purpose of this paper is precisely to calculate the resonance energies by Borel summation of the RSPT. A main point is that the Borel sum provides the imaginary part of the resonance energy, as well as the real energy shift, even though the RSPT coefficients are all real. In practice this technique is expected to fill the gap between very small field strengths, for which the simple asymptotic formula may be used directly, and large field strengths, for which variational methods work well. That is, it is expected to be more effective at moderate field strengths than variational methods.

II. BOREL-PADÉ METHOD

Let us recall the definition of the Borel sum.[28] From the given power series, which in this case we denote by

$$\sum_{N=0}^{\infty} E^{(N)}F^N , \tag{1}$$

the Borel transform is first defined by the series,

$$B(F)=\sum_{N=0}^{\infty} E^{(N)}F^N/N! \tag{2}$$

whose radius of convergence in this case[14,20,29–31] is $\frac{2}{3}n^{-3}$, where n is the principal quantum number. Second, it is necessary to find the analytic continuation of $B(F)$ for F outside the cricle of convergence. Then the Borel sum is obtained from the Borel transform via

$$E(F)=\int_0^{\infty} e^{-t}B(tF)dt , \tag{3}$$

if the integral exists. In this specific case, as proved in Ref. 26, the integral exists for F not on the real axis. This is because the real axis is a Stokes line of the asymptotic expansion (1), and to include the real axis here it is necessary to take the analytic continuation of (3):

$$E(F)=\alpha\int_0^{\infty} e^{-\alpha t}B(\alpha tF)dt , \tag{4}$$

where α is some nonreal number with $\text{Re}(\alpha)>0$, and whose exact value is not crucial. There are, in fact, two distinct analytic continuations, depending on the sign of $\arg(\alpha)$. The choice $\arg(\alpha)>0$ makes the sign of the $\text{Im}E(F)$ turn out negative. It is proved in Ref. 26 that the Borel sums $E(F)$ of Eq. (4) are the actual resonances of the LoSurdo-Stark problem with the usual sign convention for the imaginary part. In the calculations described below we took α to be $i^{1/2}$.

The practical problem in applying the Borel technique is to compute the analytic continuation of $B(F)$ beyond its circle of convergence. As suggested in Refs. 32 and 33, it is possible that this can be done via Padé approximants. It seems clear from numerical calculations that the series for the Borel transform (2) is not Stieltjes (which follows from the signs of certain determinants of matrices of the series coefficients), but nevertheless the diagonal Padé approximants for $B(\alpha tF)$ do not seem to have poles on the positive t axis for $\alpha=i^{1/2}$, which would have been the major impediment to using the Padé method. That is, even though we do not have a proof of convergence, the Padé approximants in the present, practical calculation work.

III. COMPUTATIONAL DETAILS

For the RSPT coefficients $E^{(N)}$ we used the standard method described earlier.[18,31] For the ground state (and for any state for which the parabolic quantum numbers n_1 and n_2 are equal) the series is even. [It is possible (but not proved) that the series (1) is Stieltjes as a function of $-F^2$.] We computed the Borel transform using the diagonal and $[N+1/N]$ Padé approximants on the series in $(\alpha tF)^2$ to avoid the zero terms. The calculation used the continued-fraction formula (see Refs. 33—35) for the diagonal Padé approximants. A big advantage was that the coefficients were computed only once, and evaluation of the continued fraction at specific values of αtF took almost no computer time. In principle it would have been possible to use $E^{(N)}$ through order 150. However, there was a loss in significant figures involved in calculating the higher-order determinants that enter into the formula for the continued-fraction coefficients, and in practice one could not go higher than $N=100$ in double precision on a Control Data Corporation CDC-7600 computer before all significance disappeared when the $E^{(N)}$ were calculated in single precision. We remark that the continued-fraction coefficients were not all positive, which means that the series (2) for the transform was not Stieltjes. We also remark that one could solve explicitly for the zeros of the Padé denominators and then evaluate $\mathrm{Im}E(F)$ analytically via the residue theorem. For very small field strengths (e.g., less than 0.03 a.u. for the ground state) at which $\mathrm{Im}E(F)$ becomes exponentially small, such an analytic procedure would be particularly effective.

For excited states with n_1 not equal n_2, the even and odd terms behave as if they belong to two distinct series (cf., for instance, Refs. 14, 20, and 29—31). For this reason we decided not to compute the Borel sum of the series (1) as described above, but instead to take the two subseries separately,

$$\sum_{N=0}^{\infty} E^{(2N)}F^{2N}\,, \quad \sum_{N=0}^{\infty} E^{(2N+1)}F^{2N+1}\,, \tag{5}$$

which clearly is permissible because of the linearity of the Borel method. Of course in computing the Padé approximants for the Borel transforms, we eliminated the alternating zero terms from each of the series. The results at appropriately scaled field strengths were comparable to those for the ground state (for which there are a larger number of calculations by other methods for comparison), and so the results for excited states have been omitted here.

The integral indicated in Eq. (4) was evaluated numerically by first truncating the interval $[0,\infty)$ at $t=100$, then subdividing [0,100] into as many as 101 subintervals concentrated between 0 and 20, and finally using the CERN (European Organization for Nuclear Research, Geneva) library subroutine CGAUSS to evaluate the integral over each subinterval. CGAUSS is based on the Gauss-Legendre numerical integration method and uses a

TABLE I. Comparison of complex eigenvalues for the hydrogenic 1s state in fields of 0.03—0.10 a.u. as determined by the Padé-Borel method versus complex-coordinate variational calculations and versus the sequential Padé-Padé method.

Computational method	$E(F)$ (a.u.)	
	$F=0.03$ a.u.	
Borel-Padé [13/12] (max. RSPT order 50)	$-0.502\,074\,272\,607\,1$	$-i\,0.111\,876\,462\times 10^{-7}$
Sequential Padé-Padé [12/12] (Ref. 21)	$-0.502\,074\,272\,6$	$-i\,0.111\,90\times 10^{-7}$
Complex coordinate (Ref. 22)	$-0.502\,074\,272\,6$	$-i\,0.111\,881\times 10^{-7}$
Complex coordinate (Ref 20)	$-0.502\,074\,272\,60$	$-i\,0.111\,880\times 10^{-7}$
	$F=0.04$ a.u.	
Borel-Padé [18/17] (max. RSPT order 70)	$-0.503\,771\,591\,013\,7$	$-i\,0.194\,634\,999\,5\times 10^{-5}$
Complex coordinate (Ref. 20)	$-0.503\,771\,591\,00$	$-i\,0.194\,635\times 10^{-5}$
	$F=0.05$ a.u.	
Borel-Padé [23/22] (max. RSPT order 90)	$-0.506\,105\,425\,362\,6$	$-i\,0.385\,920\,828\times 10^{-4}$
Complex coordinate (Ref. 20)	$-0.506\,105\,425\,35$	$-i\,0.385\,920\,8\times 10^{-4}$
	$F=0.06$ a.u.	
Borel-Padé [25/25] (max. RSPT order 100)	$-0.509\,203\,450\,879$	$-i\,0.257\,538\,747\times 10^{-3}$
Sequential Padé-Padé [12/12] (Ref. 21)	$-0.509\,203\,60$	$-i\,0.257\,545\times 10^{-3}$
Complex coordinate (Ref. 22)	$-0.509\,203\,45$	$-i\,0.257\,538\,9\times 10^{-3}$
Complex coordinate (Ref. 20)	$-0.509\,203\,450\,87$	$-i\,0.257\,538\,74\times 10^{-3}$
	$F=0.08$ a.u.	
Borel-Padé [25/25] (max. RSPT order 100)	$-0.517\,560\,617\,1$	$-i\,0.226\,982\,88\times 10^{-2}$
Sequential Padé-Padé [13/13] (Ref 21)	$-0.517\,559\,5$	$-i\,0.226\,865\times 10^{-2}$
Complex coordinate (Ref. 22)	$-0.517\,560\,62$	$-i\,0.226\,982\,7\times 10^{-2}$
Complex coordinate (Ref. 20)	$-0.517\,560\,617\,00$	$-i\,0.226\,982\,877\times 10^{-2}$
	$F=0.10$ a.u.	
Borel-Padé [25/25] (max. RSPT order 100)	$-0.527\,418\,176$	$-i\,0.726\,905\,6\times 10^{-2}$
Sequential Padé-Padé [12/12] (Ref. 21)	$-0.527\,425$	$-i\,0.727\,062\times 10^{-2}$
Complex coordinate (Ref. 22)	$-0.527\,418\,173$	$-i\,0.726\,905\,7\times 10^{-2}$
Complex coordinate (Ref. 20)	$-0.527\,418\,175\,09$	$-i\,0.726\,905\,676\times 10^{-2}$

minimum of 16 points per interval. The continued-fraction implementation to calculate the diagonal Padé approximants, as described above, was used by CGAUSS at each point of the numerical integration. The truncation point ($t=100$) and the subdivision of [0,100] were not completely optimized, but were determined by numerical experiment to guarantee the precision of the results as reported in the table up to but not including the last digit.

We report in Table I the real and imaginary parts of the resonance energies for the ground state for field strengths of 0.03–0.10 a.u. Also reported in Table I for comparison are values computed by other methods. It is immediately apparent that the most accurate values at the smaller field strengths listed in Table I are given by the Borel-Padé method. At the next to highest field (0.08 a.u.), the Borel-Padé value falls between the two complex-coordinate values, while at the highest field (0.10 a.u.) the complex-coordinate method gives the best result. It is possible that the Borel-Padé value at $F=0.10$ a.u. could be improved by going to a higher order, but that was not possible with the precision available. The sequential Padé-Padé values, which are the easiest to obtain, seem less accurate. That may be in part because they were not taken to as high an order. [In the light of the usefulness of the sequential Padé-Padé method, it would be very interesting if it could be proved that the RSPT series (1) is Stieltjes, which would guarantee the convergence of that method.]

IV. REMARKS

The calculations reported above demonstrate two main points. (i) The RSPT series, all the coefficients of which are real, already contain all the information to get the imaginary part of the resonance eigenvalues.[21,26,31] (ii) By calculating the Borel transform via Padé approximants, the Borel method applied to the perturbation series gives both the real and imaginary parts of the resonances to high accuracy—i.e., the Borel-Padé method is an effective, practical computational tool.

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