

# Stark effect in hydrogen: Reconstruction of the complex ground-state energy from the coefficients of an asymptotic perturbation expansion

I. A. Ivanov

*Institute of Spectroscopy, Academy of Sciences of Russia, Troitsk, Moscow Region 142092, Russia*

(Received 17 May 1996; revised manuscript received 13 February 1997)

We consider the Stark effect for the ground state of hydrogen. Using the Borel summability of the Rayleigh-Schrödinger perturbation expansion we sum it about the pure imaginary field strength  $\mathcal{E}=i\mathcal{F}$ ,  $\mathcal{F}$  is real. As a result we obtain the series converging for small values of  $\mathcal{F}$ . We give arguments that this series converges for all positive finite values of  $\mathcal{F}$ . The series obtained can be continued analytically back to the real field strength region. This method allows one to obtain accurate results for the hydrogenic Stark resonances with slight computational effort. [S1050-2947(97)07307-1]

PACS number(s): 03.65.Db

## I. INTRODUCTION

The Stark effect in hydrogen is one of the oldest quantum-mechanical problems. In the presence of the uniform electrostatic field the discrete energy levels of hydrogen shift and broaden, becoming Stark effect resonances. These resonances can be associated with complex energy eigenvalues [1–3]. The real part of such an eigenvalue is interpreted as the energy of a metastable state, the imaginary part is related to the ionization rate. The appearance of resonances can be pictured as the motion of the bound states' energy eigenvalues of hydrogen from the real axis into the lower half complex plane, with every bound state giving rise to a resonance [4].

The spectrum of the resonance energies and eigenfunctions of atomic hydrogen was investigated in a number of works. In [3] the positions and widths of the resonances were obtained by means of Breit-Wigner analysis of the continuum wave function. Popov *et al.* [5,6] used  $1/n$ -expansion method. In [7–12] the resonance eigenvalues and eigenfunctions were computed by means of complex coordinate variational methods. Alvarez, Damburg, and Silverstone [12] applied the concept of resonances for the calculation of the photoionization cross section of atomic hydrogen and reproduced the results of experiments [13,14]. In [15] the method of calculation of the resonance energies based on the rational approximation of the logarithmic derivative of the eigenfunction (Riccati-Padé method) was developed. The positions and widths of the resonances were also computed by means of direct numerical integration of the second-order differential equations [16] and power series expansions [17].

The methods mentioned above can be considered as the nonperturbative ones. Another group of methods of the calculation of the resonance energies makes use of the Rayleigh-Schrödinger perturbation expansion.

It is known [18] that consideration of the Stark effect by means of the Rayleigh-Schrödinger perturbation theory, the operator of the interaction of an atom with the electrostatic field being considered as the perturbing operator, yields a divergent asymptotic series in powers of the field strength  $\mathcal{E}$ . Despite its divergency the perturbation expansion provides information about the complex level energies of hydrogen in

the presence of the uniform electrostatic field. In [19–21] the complex Stark eigenvalues have been computed via analytic continuation of the perturbation series into the complex plane and back to the real axis, summation of the series being achieved by an application of Padé approximants. In [22] the perturbation series was continued analytically by shifting the origin of the real series into the complex plane; the resulting divergent series was summed by Padé approximants.

A powerful tool for the summation of divergent series is the Borel summation method. That the Stark problem in hydrogen is Borel summable in a suitable sense was shown in [4,23]. In these works it was shown that the perturbation series in powers of the field strength  $\mathcal{E}$  is Borel summable if the field strength  $\mathcal{E}$  assumes complex values and its sum can be afterwards continued analytically back to the real field strength region. Borel summability of the perturbation series implemented by the Borel-Padé method was used in [20] to obtain the perturbed energy and ionization rate in the presence of the uniform electrostatic field.

In [24] the concept of the distributional Borel summability was introduced. It was shown [25] that the Stark effect perturbation series possesses the property of the distributional Borel summability, and that the positions and widths of the resonances are uniquely determined from the perturbation expansion by means of the distributional Borel summation.

In the present paper we shall use the above-mentioned Borel summability (in the ordinary sense) of the Stark effect perturbation expansion for the complex values of the field strength  $\mathcal{E}$ . We propose a procedure allowing one to calculate effectively the Borel sum of the Stark effect perturbation series for the ground state of hydrogen for the pure imaginary field strength  $\mathcal{E}$ . As a result we obtain an expression that can be analytically continued back to the real field strength region and that can be used for the effective computation of the ground-state resonance eigenvalue.

## II. THEORY

The coefficients of the perturbation expansion

$$E(\mathcal{E}) \sim -\frac{1}{2} \sum_{n=0}^{\infty} E_n \left(\frac{\mathcal{E}}{4}\right)^{2n} \quad (1)$$

TABLE I. Coefficients  $f_n$ ,  $\tilde{f}_n$ ,  $g_n$  and ratios  $r_n$ .

$n$	$f_n$	$\tilde{f}_n$	$r_n$	$g_n$
0	0.261799	0.261799		0.261799
5	0.486759	0.061287	-1.325313	0.019246
10	0.725566	-0.041542	-1.014924	-0.011575
15	0.813032	0.032057	-1.064684	0.005397
20	0.857903	-0.026476	-1.020426	-0.004035
25	0.885360	0.024762	-1.015347	0.003974
30	0.903912	-0.022055	-1.027540	-0.002774

were calculated in a number of works [26–28]. In the present work we use the data from [27] where first thirty  $E_n$  were calculated for the ground state of hydrogen. All  $E_n$  are integer numbers; the first few of them are  $E_0=1$ ,  $E_1=72$ , and  $E_2=28\,440$ . The large-order perturbation coefficients  $E_n$  are known to have the following asymptotic behavior [29]:

$$E_n \sim \frac{12}{\pi} 36^n \Gamma(2n+1) \left(1 - \frac{107}{36n}\right), \quad n \rightarrow \infty. \quad (2)$$

Factorial growth of  $E_n$  is related to the Borel summability of the series (1).

Let us represent the coefficients  $E_n$  as follows:

$$E_n = \frac{12}{\pi} 36^n \Gamma(2n+1) f_n, \quad n=0,1,\dots, \quad (3)$$

where we introduced the coefficients  $f_n$ . Some of  $f_n$  are presented in the second column of the Table I. Large- $n$  asymptotic behavior of  $f_n$  can easily be found by comparing the formulas (2) and (3):  $f_n \sim 1 - 107/36n$ . Such asymptotic behavior of  $f_n$  implies that the series

$$f(z) = \sum_{n=0}^{\infty} f_n z^n \quad (4)$$

converges if  $|z| < 1$ . Moreover, since all  $f_n$  are positive, one can conclude according to the theorem by Pringsheim that  $f(z)$  has a singularity at the point  $z=1$ .

It was shown in [4,23] that the series (1) is Borel summable if the field strength  $\mathcal{E}$  assumes complex values. The sum of the series for the physical values of the field strength can be found with the help of analytical continuation to the real values of  $\mathcal{E}$ . In the next section we shall find the Borel sum of the series (1) for the pure imaginary  $\mathcal{E}$ .

#### A. Borel sum of the series (1) for the pure imaginary values of $\mathcal{E}$

Let us suppose that the field strength  $\mathcal{E}$  assumes pure imaginary value  $\mathcal{E}=i\mathcal{F}$ , where  $\mathcal{F}$  is real. Using the Borel summability of the series (1) for the imaginary values of  $\mathcal{E}$  and applying the Borel summation procedure to the series (1) one can obtain for  $E(\mathcal{E})$  the following expression:

$$E(\mathcal{E}) = -\frac{6}{\pi} \int_0^{\infty} e^{-y} f(by^2) dy, \quad (5)$$

where  $b=9\mathcal{E}^2/4=-9\mathcal{F}^2/4$ . For the case considered of the pure imaginary  $\mathcal{E}$  the parameter  $b$  is negative.

One recovers the asymptotic expansion (1) from the formula (5) if one substitutes for the function  $f(z)$  its power series expansion (4) and performs formally term-by-term integration.

We shall use the recipe of the transformation of an asymptotic series into a convergent one proposed by Loeffel [30]. It was shown in [30] that asymptotic divergent series can be transformed into a convergent one with the help of a suitable conformal mapping of a neighborhood of the positive real axis onto the unit disk, the positive real axis being mapped onto the interval  $[0,1]$ .

Let us consider the following transformation

$$by^2 = \frac{x}{1+x}, \quad (6a)$$

$$x = \frac{by^2}{1-by^2}. \quad (6b)$$

This mapping maps the interval of integration  $y \in [0, \infty)$  in Eq. (5) onto the interval  $x \in (-1, 0]$ . Knowing the coefficients  $f_n$  of the series (4) one can find the coefficients of the expansion of  $f(by^2)$  in powers of  $x$  about the point  $x=0$ :

$$f(by^2) = \tilde{f}(x) = \sum_{n=0}^{\infty} \tilde{f}_n x^n. \quad (7)$$

We computed  $\tilde{f}_n$  using the exact rational arithmetic of MATHEMATICA. As the coefficients  $f_n$  divided by  $\pi$  are rational numbers we were able to compute first thirty  $\tilde{f}_n$  exactly. Some of them are presented in the third column of the Table I. (We present them as decimals to save space.)

The radius of convergence of the series (7) is determined by the nearest to the  $x=0$  singular point of  $\tilde{f}(x)$ . As we have seen, the function  $f(z)$  has a singular point at  $z=1$ . The mapping (6) maps this point onto the point  $x=\infty$  of the  $x$  complex plane. Therefore, the radius of convergence of the series (7) is determined by some other singular point of the function  $\tilde{f}(x)$ . To find the position of this singular point we performed a ratio test, that is, we computed the sequence of the following ratios  $r_n = \tilde{f}_{n-1}/\tilde{f}_n$ . Some  $r_n$  are presented in the fourth column of Table I. It is well known that the limit of this sequence is equal to  $R$ —the radius of convergence of the series (7). The data from Table I indicate that  $R \approx 1$ . We make an assumption that  $R=1$  exactly. This assumption is justified by the correctness of the result for the energy we shall obtain below. As the series (7) is a sign-alternating one, the singular point  $x_s$  determining  $R$  is on the negative real axis (we used the theorem by Pringsheim). Therefore,  $\tilde{f}(x)$  has a singular point at  $x=-1$ . According to the formulas (6) this implies that  $f(z)$  has a singular point at  $z=\infty$ . The nature of this singular point was difficult to study numerically, as we had a relatively small number of the coefficients  $f_n$  at our disposal.

One can make some guesses about the nature of a singular point of  $f(z)$  when  $z \rightarrow \infty$  using information about the large field asymptotic behavior of the Stark resonances [9,31]. The leading-order large field asymptotic behavior of the complex

energy eigenvalue is given by the formula  $|E(\mathcal{E})| \sim \frac{1}{2}[\frac{1}{2}\mathcal{E} \ln(\mathcal{E})]^{2/3}$ . From Eq. (5) one can see that in order to reproduce such asymptotic behavior the function  $f(z)$  should behave as  $z^{1/3} \ln^{2/3} z$  for large  $z$  values. This implies that in the  $x$  complex plane, the function  $\tilde{f}(x)$  may be expected to have a singular point of the type  $(1+x)^{-1/3} \ln^{2/3}(1+x)$  at the point  $x = -1$ . To single out the leading singular behavior of  $\tilde{f}(x)$ , we represent this function as

$$\tilde{f}(x) = \frac{g(x)}{(1+x)^{1/3}}. \quad (8)$$

The function  $g(x)$  can be expanded in a power series about the point  $x=0$ :

$$g(x) = \sum_{n=0}^{\infty} g_n x^n. \quad (9)$$

All  $g_n$  are rational numbers and were computed exactly with the help of the exact rational arithmetic of MATHEMATICA. Some  $g_n$  values are presented in the fifth column of Table I. Numerical study of  $g_n$  indicates that the function  $g(x)$  is still singular at the point  $x = -1$ , but has there less severe singularity than  $\tilde{f}(x)$ . This numerical observation corresponds to the above-presented discussion of the properties of  $\tilde{f}(x)$  from which it follows that  $g(x)$  may be expected to have a logarithmic singularity at the point  $x = -1$ .

Using Eqs. (7)–(9) one obtains for the function  $f(by^2)$  from Eq. (5) the following formula:

$$f(by^2) = (1-by^2)^{1/3} \sum_{n=0}^{\infty} (-1)^n g_n \left(-\frac{by^2}{1-by^2}\right)^n. \quad (10)$$

We recall that the parameter  $b$  in Eq. (10) is negative for the pure imaginary values of the field strength  $\mathcal{E}$ . Substituting expansion (10) into the formula (5) and performing term-by-term integration (the justification of this operation will be given below) we obtain the following formula for  $E(\mathcal{E})$ :

$$E(\mathcal{E}) = -\frac{6}{\pi} \left(\frac{9\mathcal{F}^2}{4}\right)^{1/3} \sum_{n=0}^{\infty} (-1)^n g_n I_n, \quad (11)$$

where for the integrals  $I_n$  we have [36]

$$\begin{aligned} I_n = & \int_0^{\infty} e^{-y} \frac{y^{2n}}{(y^2+4/9\mathcal{F}^2)^{n-1/3}} dy = \Gamma\left(\frac{5}{3}\right) {}_1F_2\left(n-\frac{1}{3}; \frac{1}{6}, \right. \\ & \left. -\frac{1}{3}; -\frac{1}{9\mathcal{F}^2}\right) + \frac{1}{2} \left(\frac{2}{3\mathcal{F}}\right)^{5/3} B\left(-\frac{5}{6}, n+\frac{1}{2}\right) \\ & \times {}_1F_2\left(n+\frac{1}{2}; \frac{1}{2}, \frac{11}{6}; -\frac{1}{9\mathcal{F}^2}\right) - \frac{1}{2} \left(\frac{2}{3\mathcal{F}}\right)^{8/3} \\ & \times B\left(-\frac{4}{3}, n+1\right) {}_1F_2\left(n+1; \frac{3}{2}, \frac{7}{3}; -\frac{1}{9\mathcal{F}^2}\right). \quad (12) \end{aligned}$$

In this equation  $B(x,y)$  is the Euler beta function and the function  ${}_1F_2(a; b_1, b_2; z)$  is given by the following hypergeometric series converging for all  $z$ :

$${}_1F_2(a; b_1, b_2; z) = \sum_{i=0}^{\infty} \frac{(a)_i}{(b_1)_i (b_2)_i} \frac{z^i}{i!}, \quad (13a)$$

where  $(a)_i = \Gamma(a+i)/\Gamma(a)$  is the Pochhammer symbol. The function  ${}_1F_2(a; b_1, b_2; z)$  can also be expressed in terms of Meyer  $G$  functions [35]:

$${}_1F_2(a; b_1, b_2; z) = \frac{\Gamma(b_1)\Gamma(b_2)}{\Gamma(a)} G_{1,3}^{1,1}\left(x \left| \begin{matrix} 1-a \\ 0, 1-b_1, 1-b_2 \end{matrix} \right. \right). \quad (13b)$$

In our calculations we used the power series representation (13a). Since the series (13a) converges everywhere in the  $z$  complex plane and all parameters of the hypergeometric functions in Eq. (12) are rational numbers one can calculate the sum of the series (13a) with arbitrarily high accuracy with the help of the exact rational arithmetic of MATHEMATICA.

We recall that the formulas (11) and (12) were obtained for the pure imaginary values of the field strength  $\mathcal{E} = i\mathcal{F}$ ,  $\mathcal{F}$  is real. When deriving Eq. (11) we assumed that the series (10) could be integrated term by term. To justify this assumption we refer to the known theorem [34] stating that if the terms of a given series are all positive and continuous functions, the sum of the series is a continuous function too, and if the series of obtained as a result of the formal term-by-term integration converges, then the given series can be integrated term by term. The requirements of the continuity

TABLE II. Partial sums of the series (11) for the pure imaginary values of  $\mathcal{E}$  (in a.u.).

$n$	$E_n(\mathcal{E})$			
	$\mathcal{E}=0.03i$	$\mathcal{E}=0.05i$	$\mathcal{E}=0.1i$	$\mathcal{E}=0.5i$
5	-0.49801684719911782	-0.4946656671696	-0.4808687192	-0.2868989877
10	-0.49801684699494024	-0.4946656417809	-0.4808634930	-0.2795301817
20	-0.49801684699471971	-0.4946656415334	-0.4808631466	-0.2759808948
30	-0.49801684699471969	-0.4946656415331	-0.4808631405	-0.2751851178
	$\mathcal{E}=3i$	$\mathcal{E}=5i$	$\mathcal{E}=10i$	$\mathcal{E}=100i$
5	0.5834859836	1.0194151787	1.8322678062	9.1275822602
10	0.7618152373	1.3177935785	2.3678127667	11.831778057
20	0.9263495187	1.6123476904	2.9248180317	14.762749606
30	1.0081384659	1.7714866727	3.2461563264	16.548049504

TABLE III. Partial sums of the series (11) for the real and imaginary parts of  $E(\mathcal{E})$  (in a.u.) for different values of the field strength, compared with other results.

$\mathcal{E}$ (a.u.)	$n$	Re $E_n(\mathcal{E})$	Re $E(\mathcal{E})_{\text{other}}$	Im $E_n(\mathcal{E})$	Im $E(\mathcal{E})_{\text{other}}$
0.025	10	-0.50142929183356		$-0.128270 \times 10^{-9}$	
	20	-0.50142929181825		$-0.166452 \times 10^{-9}$	
	28	-0.50142929181836	-0.50142929180 <sup>a</sup>	$-0.165918 \times 10^{-9}$	
	30	-0.50142929181840	-0.501429291818 <sup>b</sup>	$-0.165940 \times 10^{-9}$	$-0.165645 \times 10^{-9b}$
0.03	10	-0.50207427299798		$-0.118549 \times 10^{-7}$	
	20	-0.50207427261640	-0.50207427260 <sup>c</sup>	$-0.111744 \times 10^{-7}$	
	28	-0.50207427260811	-0.502074272604 <sup>b</sup>	$-0.111891 \times 10^{-7}$	$-0.111880 \times 10^{-7c}$
	30	-0.50207427260806	-0.5020742726071 <sup>d</sup>	$-0.111876 \times 10^{-7}$	$-0.111876462 \times 10^{-7c}$
0.05	10	-0.5061058109		$-0.38787 \times 10^{-4}$	
	20	-0.5061054390	-0.50610542535 <sup>c</sup>	$-0.38613 \times 10^{-4}$	
	28	-0.5061054239	-0.5061054253626 <sup>d</sup>	$-0.38588 \times 10^{-4}$	$-0.3859208 \times 10^{-4c}$
	30	-0.5061054230	-0.5061054243 <sup>b</sup>	$-0.38591 \times 10^{-4}$	$-0.386013 \times 10^{-4b}$
0.1	10	-0.5275107		-0.0072826	
	20	-0.5274024		-0.0072726	
	28	-0.5274207	-0.52741817509 <sup>c</sup>	-0.0072727	$-0.00726905676^c$
	30	-0.5274212	-0.5274213 <sup>b</sup>	-0.0072705	$-0.00726637^b$
0.5	10	-0.64230		-0.31986	
	20	-0.64598		-0.28036	
	28	-0.63460	-0.6230680256 <sup>e</sup>	-0.27059	$-0.279744825^e$
	30	-0.63228	-0.620997 <sup>b</sup>	-0.26984	$-0.279793^b$
1	10	-0.47016		-0.74026	
	20	-0.58482		-0.75414	
	28	-0.63129	-0.62433650736 <sup>c</sup>	-0.73186	$-0.64682090008^c$
	30	-0.63825	-0.626236 <sup>b</sup>	-0.72618	$-0.635644^b$
10	10	1.18210		-2.41180	
	20	1.43623		-3.04093	
	28	1.54820	0.6082717056 <sup>e</sup>	-3.37793	$-5.578015929^e$
	30	1.56737	0.60827170547 <sup>c</sup>	-3.44168	$-5.5780159282^c$
1000	10	27.5274		-47.6828	
	20	34.3646		-59.5275	
	28	37.8847		-65.6264	
	30	38.5406	81.848982715 <sup>c</sup>	-66.7628	$-189.25530177^c$

<sup>a</sup>Reference [33].

<sup>b</sup>Reference [23].

<sup>c</sup>Reference [9].

<sup>d</sup>Reference [32].

<sup>e</sup>Reference [15].

are fulfilled in our case. To fulfill the requirement of positivity the series  $\sum g_n$  must be a sign-alternating one. The fact that the function  $g(x)$  has a singularity at  $x = -1$  and numerical evidence (the data are presented in the fifth column of the Table I) support the hypothesis that  $\sum g_n$  is a sign-alternating series. Consider the last condition of the theorem we cited above. The large- $n$  asymptotic of the integrals  $I_n$  in Eq. (11) can be obtained with the help of the saddle-point method. One obtains

$$I_n \sim \left(\frac{8}{9}\right)^{8/9} \left(\frac{3\pi}{4}\right)^{1/2} \frac{n^{7/18}}{\mathcal{F}^{7/9}} \exp\left[-\left(\frac{3}{\mathcal{F}^2}\right)^{1/3} n^{1/3}\right]. \quad (14)$$

For  $n \rightarrow \infty$   $I_n$  decay exponentially. If the coefficients  $g_n$  slowly decrease in magnitude when  $n \rightarrow \infty$  (or at least if their growth is slower than exponential) the series on the right-hand side of the Eq. (11) converges for any positive real

value of  $\mathcal{F}$ . We have reason to believe that the coefficients  $g_n$  do decay slowly when  $n \rightarrow \infty$ . Our arguments are based on the properties of the function  $g(x)$  we have discussed above. Indeed, if, as we supposed, the function  $g(x)$  has a mild (logarithmic) singularity at  $x = -1$  then the coefficients  $g_n$  form a sequence slowly decreasing in magnitude. We were unable to prove this hypothesis rigorously. Numerical evidence strongly supports its validity. Below, we shall assume that this hypothesis is true. Then, all the conditions of the theorem we cited above are fulfilled and the expansion (10) can be integrated term by term. Asymptotic (14) of  $I_n$  and supposed slow decrease of  $g_n$  allow one to conclude that the series (11) converges for any positive finite  $\mathcal{F}$ . Moreover convergence is uniform for any compact  $\mathcal{F} \in [\alpha, \beta]$ ,  $\alpha, \beta$  being positive finite numbers. In the interval  $\mathcal{F} \in (0, \infty)$  the convergence is nonuniform. This observation helps to resolve a seeming contradiction between true asymptotic behavior of

$E(\mathcal{F})$  for  $\mathcal{F} \rightarrow \infty$  (the leading term of asymptotic behavior is  $E(\mathcal{F}) \sim \frac{1}{2} [\frac{1}{2} \mathcal{F} \ln(\mathcal{F})]^{2/3}$  [9,31]) and asymptotic behavior given by Eq. (11) if one passes formally to the limit  $\mathcal{F} \rightarrow \infty$  under the summation sign in Eq. (11). If in Eq. (12) we put formally  $\mathcal{F} = \infty$ , the series on the right-hand side of Eq. (11) reduces to the series  $\sum (-1)^n g_n$ . For  $g(x)$  having a logarithmic singularity at  $x = -1$ , this series is divergent. Therefore, the passage to the limit  $\mathcal{F} \rightarrow \infty$  under the summation sign in Eq. (11) is not legitimate.

To illustrate the convergence properties of the series (11) we present in the Table II the partial sums of the series (11) for the pure imaginary values of the field strength  $\mathcal{E} = i\mathcal{F}$ , where  $\mathcal{F}$  is real. For the small values of  $\mathcal{F}$  ( $\mathcal{F} \leq 0.05$  a.u.) the convergence of the series (11) is apparent and very rapid. The convergence of the series (11) for the small values of  $\mathcal{F}$  gives us strong numerical evidence that our hypothesis about slow decay or at least not very fast growth of the coefficients  $g_n$  is true, but then the series (11) converges for any positive finite value of  $\mathcal{F}$ . As one can see from Table II for the large values of  $\mathcal{F}$  the convergence is rather slow. This circumstance is in agreement with the asymptotic estimation (14) of the integrals  $I_n$ .

To obtain the physical results one should continue analytically the sum of the series (11) back to the real field strength region.

### B. Analytic continuation to the real field strength region

We are going to show that the series (11) can be continued analytically to  $\mathcal{E}$  real. For  $\mathcal{E}$  real, the parameter  $\mathcal{F}$  in Eqs. (11) and (12) is pure imaginary  $\mathcal{F} = -i\mathcal{E}$ . One can show that the asymptotic behavior of  $I_n$  for the imaginary values of  $\mathcal{F}$  is given by the same formula (14) as in the case of real  $\mathcal{F}$ . Therefore, for any real positive finite  $\mathcal{E}$   $I_n$  decay for sufficiently large  $n$  as  $e^{-an^{1/3}}$  with  $\text{Re}(a) > 0$ .

Therefore, if the series (11) converges for pure imaginary  $\mathcal{E}$ , it will be converging for real  $\mathcal{E}$ , and will provide the desired analytical continuation of  $E(\mathcal{E})$ . This analytical continuation is achieved simply by putting  $\mathcal{F} = -i\mathcal{E}$  in the formulas (11) and (12).

In Table III we present the sequence of the partial sums of the series (11) for the real and imaginary parts of energy calculated for the different values of the field strength. These data are compared with other results. One can see that the convergence for the real part of energy is excellent for the small values of the field strength ( $\mathcal{E} < 0.05$  a.u.). Account of the first 30 terms of the series (11) yields about 12 digits of

the exact result for  $E(\mathcal{E})$ . As far as the imaginary part of energy is concerned, convergence is not so good. A relatively poor convergence for the imaginary part of energy for very small values of  $\mathcal{E}$  is not surprising if one takes into account extremely singular behavior of  $\text{Im}(E)$  for small  $\mathcal{E}$ . In this limit the behavior of the imaginary part of energy is described by the well-known semiclassical formula  $\text{Im}(E) \sim 2\mathcal{E}^{-1} \exp(-2/3\mathcal{E})$ . For  $\mathcal{E} < 0.05$  a.u. the first 30 terms of the series (11) give about four digits of the exact result for the imaginary part of energy.

For the larger values of  $\mathcal{E}$  ( $\mathcal{E} > 0.5$  a.u.), the series (11) converges more slowly as our results from Table III indicate. However, using the same arguments we used above when discussing the convergence properties of the series (11) for the pure imaginary field strength, we can assert that the series (11) converges for all positive finite values of  $\mathcal{E}$ . Indeed, as we saw, convergence properties of the series (11) are related to the large- $n$  asymptotic of the coefficients  $g_n$ . Since the integrals  $I_n$  decay exponentially for any positive finite value of  $\mathcal{E}$ , one can deduce that if the series (11) converges for the small values of the field strength  $\mathcal{E}$  it will be converging for all positive finite  $\mathcal{E}$ .

### III. REMARKS AND PROSPECTS

The key assumption that was made in the present paper was an assumption about slow decrease (or at least not very fast growth) of the absolute value of the coefficients  $g_n$ . We were unable to prove this hypothesis rigorously. However, numerical results show that it is almost certainly true. Rigorous proof of this hypothesis would be highly desirable.

As far as the questions of the computational character are concerned, the present procedure requires only a slight computational effort. For the small values of the field strength ( $\mathcal{E} < 0.03$  a.u.) an account of the first 30 terms of the series (11) yields about 12 digits of the exact result for an energy.

For the larger values of  $\mathcal{E}$  a naive direct summation of the first 30 terms of the series (11) cannot yield accurate results and one should compute more coefficients of the series (11) or employ some suitable method of the acceleration of convergence.

### ACKNOWLEDGMENT

The financial support from the Russian Foundation of Fundamental Research (Project Code 95-02-04534a) is acknowledged.

- 
- [1] A. F. J. Siegert, Phys. Rev. **56**, 750 (1939).  
 [2] B. Simon, Ann. Math. **97**, 247 (1973).  
 [3] R. J. Damburg and V. V. Kolosov, J. Phys. B **9**, 3149 (1976).  
 [4] S. Graffi and V. Grecchi, Commun. Math. Phys. **62**, 83 (1978).  
 [5] V. S. Popov, V. D. Mur, A. V. Sergeev, and V. M. Weinberg, Phys. Lett. A **149**, 418 (1990).  
 [6] V. S. Popov, V. D. Mur, and A. V. Sergeev, Phys. Lett. A **149**, 418 (1990).  
 [7] W. P. Reinhardt, Int. J. Quantum Chem. Symp. **10**, 359 (1976).  
 [8] E. Brandas and P. Froelich, Phys. Rev. A **16**, 2207 (1977).  
 [9] L. Benassi and V. Grecchi, J. Phys. B **13**, 911 (1980).  
 [10] A. Maquet, S.-I. Chu, and W. P. Reinhardt, Phys. Rev. A **27**, 2946 (1983).  
 [11] D. A. Telnov, J. Phys. B **22**, L399 (1989).  
 [12] G. Alvarez, R. J. Damburg, and H. J. Silverstone, Phys. Rev. A **44**, 3060 (1991).  
 [13] T. Bergeman, C. Harvey, K. B. Butterfield, H. C. Bryant, D. A. Clark, P. A. M. Gram, D. MacArthur, M. Davis, J. B.

- Donahue, J. Dayton, and W. W. Smith, Phys. Rev. Lett. **53**, 775 (1984).
- [14] H. Rottke and K. H. Welge, Phys. Rev. A **33**, 301 (1986).
- [15] F. M. Fernandez, Phys. Rev. A **54**, 1206 (1996).
- [16] O. Hirschfelder and L. A. Curtis, J. Chem. Phys. **55**, 1395 (1971).
- [17] M. H. Alexander, Phys. Rev. **178**, 34 (1969).
- [18] E. C. Titchmarsh, *Eigenfunction Expansions Associated with Second-Order Differential Equations* (Oxford University Press, London, 1958).
- [19] W. P. Reinhardt, Int. J. Quantum Chem. **21**, 133 (1982).
- [20] V. Franceschini, V. Grecchi, and H. J. Silverstone, Phys. Rev. A **32**, 1338 (1985).
- [21] H. J. Silverstone, Int. J. Quantum Chem. **29**, 261 (1986).
- [22] J. N. Silverman and C. A. Nicolaides, Chem. Phys. Lett. **153**, 61 (1988).
- [23] I. W. Herbst and B. Simon, Phys. Rev. Lett. **41**, 67 (1978).
- [24] E. Caliceti, V. Grecchi, and M. Maioli, Commun. Math. Phys. **104**, 163 (1986).
- [25] E. Caliceti, V. Grecchi, and M. Maioli, Commun. Math. Phys. **157**, 347 (1993).
- [26] H. J. Silverstone, B. G. Adams, J. Cizek, and P. Otto, Phys. Rev. Lett. **43**, 1498 (1979).
- [27] V. Privman, Phys. Rev. A **22**, 1833 (1980).
- [28] R. F. Stebbings, Science **193**, 537 (1976).
- [29] L. Benassi, B. Grecchi, E. Harell, and B. Simon, Phys. Rev. Lett. **42**, 704, 1430(E) (1979).
- [30] J. J. Loeffel, in *Large-Order Behavior of Perturbation Theory*, edited by J. C. Le Guillou and J. Zinn-Justin (North-Holland, Amsterdam, 1990), pp. 524–526.
- [31] G. Alvarez and H. J. Silverstone, Phys. Rev. A **50**, 4679 (1994).
- [32] M. Hehenberger, H. V. McIntosh, and E. Brändas, Phys. Rev. A **10**, 1494 (1974).
- [33] J. N. Silverman and J. Hinze, Chem. Phys. Lett. **128**, 466 (1986); Phys. Rev. A **37**, 1208 (1988).
- [34] G. M. Fikhtengolts, *Lekcii po differentsialnomu i integralnomu ischisleniyu* (Fizmatgiz, Moscow, 1962).
- [35] *Tables of Integrals, Series and Products*, edited by I. S. Gradshteyn and I. M. Ryzhik (Academic Press, New York, 1965).
- [36] *Integrali i ryadi*, edited by A. P. Prudnikov, Y. A. Brichkov, and O. I. Marichev (Nauka, Moscow, 1981).