Appl. Phys. B 78, 817–820 (2004)
DOI: 10.1007/s00340-004-1457-y

Applied Physics B
Lasers and Optics

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AC Stark shift of the ground state of atomic hydrogen

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Received: 27 October 2003/
Revised version: 24 December 2003

ABSTRACT An analytical expression for the second-order AC Stark shift of the ground state of atomic hydrogen is derived, which is convergent for negative as well as for positive energies of intermediate states except for the resonances. To clarify the applicability of the second-order perturbation theory, we compared results with those which are obtained by us and other authors using nonperturbative methods. It appears that values obtained for the AC Stark shift using our simple formula agree on average with Floquet-method calculations up to the field strength $F = 0.12$ (a.u.), which corresponds to $I = 10^{15}\ \mathrm{W/cm^2}$.

PACS 42.50.Hz; 31.15.Md

1 Introduction

In experiments with atoms exposed to a strong laser field it is observed that the atomic resonances are field shifted, which means that the atomic levels are AC field shifted. The second-order level shift for atomic hydrogen was previously calculated by Gontier and Trahin [1] by solving a system of second-order differential equations. Arnous et al. [2] used the Green's function formalism. They used a Coulomb Green's function (CGF) Sturmian expansion, which is convergent for negative energies of intermediate states. Therefore, in the case when the intermediate states are in the continuum, they applied Padé approximants. Pan et al. [3] calculated the shift of the ground state at up to the 20th order by solving the system of differential equations only for the cases when the intermediate states are in the discrete spectrum ($\lambda = 530$ nm and 1064 nm). We present a closed form for the second-order energy shift of the ground state, which may be used to calculate the shift of the $1\,s$ state at negative as well as at positive energies of intermediate states except for the resonances.

2 Closed form for the second-order AC Stark shift

In the length gauge the second-order shift of the ground state for the monochromatic electric field $F\cos\omega t$ is given by the expression

$$\Delta^{(2)}_{1\,s} = \delta E^{(2)}_{1\,s} - \mathrm{i}\Gamma^{(2)}_{1\,s} = -\frac{I}{I_0}\alpha^{(2)}_{1\,s}(\omega) = -\frac{F^2}{4F_0^2}\alpha^{(2)}_{1\,s}(\omega), \tag{1}$$

where $\Delta^{(2)}_{1\,s}$ is the second-order complex level shift.

Its real part $\delta E^{(2)}_{1\,s}$ is the energy shift and its imaginary part $\Gamma^{(2)}_{1\,s}$ gives the level width. $\alpha^{(2)}_{1\,s}(\omega)$ is the dipole dynamic polarizability. F is the field strength and I is the laser intensity expressed in a.u. The atomic units for these are $F_0 = \mathrm{e}/a_0^2 = 5.142\times10^9\ \mathrm{V/cm}$ and $I_0 = 1.4038\times10^{17}\ \mathrm{W/cm^2}$, respectively.

The level shift depends on the intensity and the frequency of the radiation. In the zero-field limit the AC shift reduces to zero. The dipole dynamic polarizability may be expressed as

$$\alpha^{(2)}_{1\,s}(\omega) = -\left[T(1\,s;\, E_{1\,s}-\omega) + T(1\,s;\, E_{1\,s}+\omega)\right], \tag{2}$$

where $T(1\,s;\,\Omega)$ is the transition amplitude, ω is the energy of a photon, and $\Omega = E_{1\,s} \mp \omega$ is the energy of intermediate states.

For the 'emission–absorption' term the energy of intermediate states is $E_{1\,s} - \omega < 0$, but for the 'absorption–emission' term it is $E_{1\,s} + \omega$. The sign of $E_{1\,s} + \omega$ depends on the location of the intermediate states: if they are in the discrete spectrum $E_{1\,s} + \omega < 0$ but if they are in the continuum $E_{1\,s} + \omega > 0$.

We obtained an expression for the diagonal two-photon transition amplitude (see Appendix A), which is valid for negative as well as positive energies of the intermediate states. In the case of linearly polarized light it has the form

$$\begin{aligned} T(1\,s;\, E_{1\,s}\pm\omega) = {} & -\frac{2^{11}}{p^3(2-p)\,(1+1/p)^{10}(1-x^2)^5} \\ & \times\sum_{m=0}^{1}\frac{(-1)_m(-1)_m(c)_m}{m!(4)_m(c+1)_m}(1-x)^{2m} \\ & \times\sum_{s=0}^{2}\frac{(c+m)_s(-2+2m)_s x^s}{s!(c+1+m)_s} \\ & \times F(1, c_1-5;\, c_1+1;\, x^2), \end{aligned} \tag{3}$$

where $x = (p-1)/(1+p)$, $|x| \le 1$, $c = 2-p$, and $c_1 = 2-p+m+s$.

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For $\Omega < 0$ we have real values for $p = (-2\Omega)^{-1/2}$. If the intermediate states are in the continuum $\Omega > 0$ and $p = -\mathrm{i}/k$, where $k = (2\Omega)^{1/2} > 0$.

The first step to obtain (3) is to use a CGF Sturmian expansion, which converges only for $\Omega < 0$. The obtained transition amplitude has an infinite summation over polynomials and needs analytical continuation to the region with $\Omega > 0$. As in [4, 5], we make a resummation to obtain a finite sum over Gauss hypergeometric functions, which are infinite sums but have well-known transformation formulae. In our case the argument of the Gauss functions $|x^2| \leq 1$. We have to use the simplest Gauss-function transformations to obtain (3). It converges not only for $\Omega < 0$ when the argument of the Gauss functions $|x^2| < 1$ but also for $\Omega > 0$ when the argument $x^2 = 1$.

In the limit of zero frequency the dynamic dipole polarizability reduces to the static dipole polarizability, which for the 1 s state is equal to $\frac{9}{2}$. For a DC field $\omega = 0$, $\Omega = E_{1s}$, and $p = 1$, so (3) simplifies and for the static dipole polarizability we obtain

$$\alpha^{(2)}_{1s}(0) = 4\sum_{m=0}^{1}\frac{(-1)_m(-1)_m(1)_m}{m!(4)_m(2)_m} = \frac{9}{2}. \tag{4}$$

3 Results and conclusions

The nonperturbative Floquet approach allows one to evaluate the level shifts correctly at much higher intensities than using perturbation theory. In Fig. 1 we present our results for Re E_{1s} dependent on the field strength calculated in the velocity gauge at $\omega = 0.184$ a.u. In the Floquet approach the radial differential equations are integrated numerically. To transform results obtained by (1)–(3) to the velocity gauge we applied the equation that shows how the level shift in the velocity gauge is expressed by the level shift in the length gauge:

$$E_{\text{velocity}} = E_{\text{length}} - E_{\text{p}}, \tag{5}$$

where $E_{\text{p}} = \frac{1}{4}F^2\omega^{-2}$ is the ponderomotive energy (i.e. the average kinetic energy of a free electron oscillating in an electromagnetic field). Comparison of results obtained using (1)–(3) and (5) to calculate δE_{1s} with those obtained by us using the Floquet method shows a good agreement up to an intensity of 10^{15} W cm^{-2}. In Figs. 2–4 we compare our results obtained using second-order perturbation theory (3) for $\Delta^{(2)}_{1s}$ with results obtained by Chu and Cooper [6] using the Floquet method and Shakeshaft and Tang [7] for five different field strength values: 0.014, 0.035, 0.071, 0.106, and 0.14 a.u., which correspond to the radiation intensities: 7.02×10^{12}, 4.39×10^{13}, 1.75×10^{14}, 3.95×10^{14}, and 7.02×10^{14} W/cm^2. Shakeshaft and Tang [7] have developed a nonperturbative integral equation method to treat the field-induced shift and width of the ground-state energy. They made calculations in the velocity gauge at some of the frequencies and intensities at which evaluations were done by Chu and Cooper [6] who used the length gauge. The agreement between the results obtained by us and others [6, 7] using the Floquet method and those obtained by us in the second-order perturbation theory using (3) are the best if the energy of

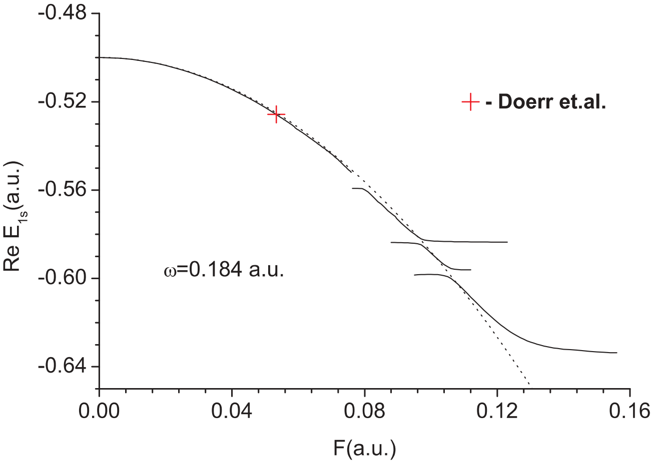

FIGURE 1 *Solid curve:* our values obtained using the Floquet method (velocity gauge), $E_{1s} \pm 7\omega$; the total basis consists of 88 functions; + the value obtained by Dörr et al. [8] using the Floquet approach; *dotted curve:* our values obtained using (3), (5)

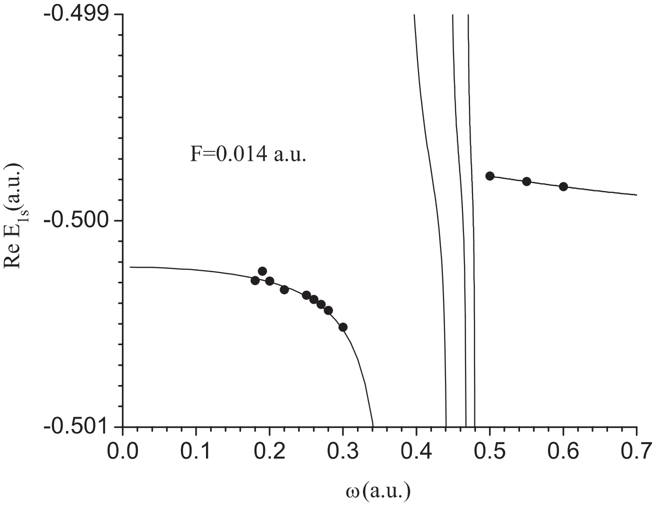

FIGURE 2 *Dots:* Floquet method, Chu and Cooper [6] (length gauge); *solid curve:* our values obtained in the second-order perturbation approximation using (3)

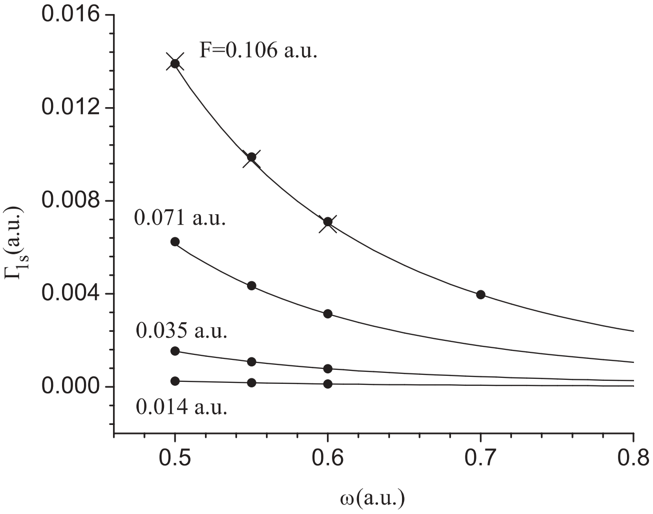

FIGURE 3 *Dots:* Floquet method, Chu and Cooper [6] (length gauge); ×: Shakeshaft and Tang [7]; *solid curve:* our values obtained in the second-order perturbation approximation using (3)

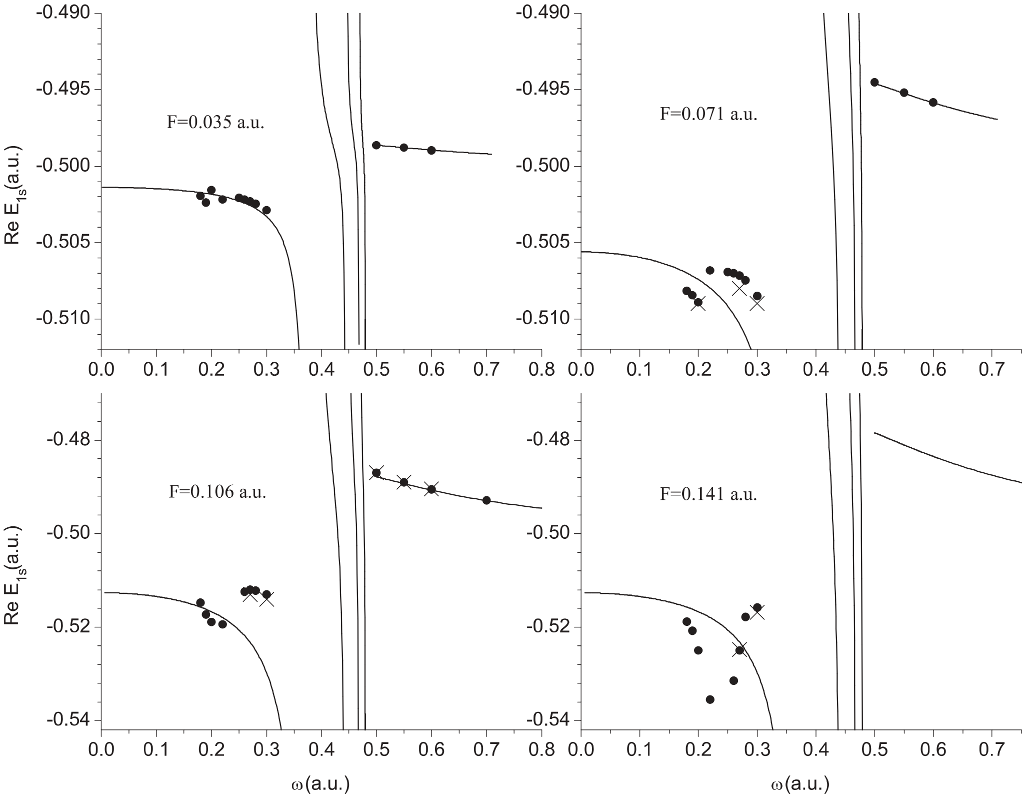

FIGURE 4 Shift of the energy of the ground state dependent on the field strength and the frequency. *Dots:* Floquet method, Chu and Cooper [6] (length gauge); ×: values obtained by Shakeshaft and Tang [7]; *solid curve:* our values obtained in the second-order perturbation approximation using (3)

a photon is enough for one-photon ionization, as in this case there are no resonances. In the case when the energy of a photon is less than the ionization potential we have the resonances and one may talk only about the average agreement of results. It is rather good up to the field strength $F = 0.12$ a.u. (Fig. 1), which corresponds to the radiation intensity $I = 10^{15}\ \mathrm{W/cm^2}$.

Appendix A

In the dipole approximation the radial part of the diagonal two-photon transition amplitude may be written in the form

$$T_{\mathrm{r}}(1\,s;\,\Omega) = 4\int_0^\infty \mathrm{d}r_1 r_1^3 \mathrm{e}^{-r_1} \int_0^\infty \mathrm{d}r_2 G_1(r_1, r_2;\,\Omega) r_2'^3 \mathrm{e}^{-r_2}, \tag{A.1}$$

where G_1 is the radial part of the Coulomb Green's function (CGF) with orbital momentum equal to unity.

The expansion of the CGF over the Sturmian basis [9] is convergent for $\Omega < 0$ and for G_1 reads explicitly

$$G_1(r_1, r_2;\,\Omega) = \sum_{n=2}^{\infty} \frac{S_{n1}(2r_1/p)S_{n1}(2r_2/p)}{1 - n/p}. \tag{A.2}$$

In the CGF Sturmian expansion the radial variables separate and it has only one infinite summation. S_{n1} are the radial components of Sturmian functions [10], which form a complete set of functions and may be written as follows:

$$S_{n1}(2r/p) = \left(\frac{2}{p}\right)^2 \sqrt{\frac{(n-2)!}{(n+1)!}} \exp(-r/p) r L_{n-2}^3(r), \tag{A.3}$$

where $p = (-2\Omega)^{-1/2}$ and $L_{n-2}^3(r)$ are Laguerre polynomials [11].

For $\Omega < 0$ the Sturmian wave functions are exponentially decreasing and therefore the infinite summation in the CGF Sturmian expansion is convergent. For $\Omega > 0$, $p = -\mathrm{i}/k$, so the Sturmian wave functions are oscillating and the infinite sum in (A.2) diverges.

We perform analytical continuation in a slightly different way from that in [4]. Inserting (A.2) in (A.1) we first carry out the integration over both angular and radial variables. So, the expression for the transition amplitude is obtained in the form

$$T(1\,s;\,\Omega) = C\sum_{n=0}^{\infty} \frac{(4)_n[{}_2F_1(-n, -1;\,4;\,1-x^{-1})x^n]^2}{n!(n+2-p)}, \tag{A.4}$$

where $x = (p-1)/(p+1)$ and $C = -2^{11}/\left[p^3(1+1/p)^{10}\right]$.

In the transition amplitude (9) there is an infinite sum over polynomials, which is not possible to continue analytically in a straightforward manner.

Transforming the denominator into an integral form $(n + 2 - p)^{-1} = \int_0^1 \mathrm{d}t\, t^{n+1-p}$, the resummation of hypergeometric functions can be performed. After some rather lengthy transformations the transition amplitude is obtained in a form of a finite sum over hypergeometric functions, which are not polynomials and have argument $|x^2| \le 1$. For $\Omega > 0$ we have $|x^2| = 1$, which means that we are on the edge of the radius of convergence for hypergeometric functions. Therefore, to obtain the convergent hypergeometric functions only the simplest transformation formula is needed:

$$_2F_1(6, c_1; c_1+1; x^2) = (1-x^2)^{-5}\,{}_2F_1(1, c_1-6; c_1+1; x^2), \tag{A.5}$$

where $c_1 = 2 - p + m + s$. So, the transition amplitude (3) is obtained, which is convergent for negative as well as positive energies except for $p = 2, 3, \ldots, n$, which correspond to the resonances in the discrete spectrum.

A similar method is used in the case of ionization with an extra photon [5], but the radial integrals in this case are more complicated, as one has intermediate states as well as the final state in the continuum. Therefore, the argument of the hypergeometric functions is in modulus greater than unity and for analytical continuation of the hypergeometric functions one has to use more complicated transformation formulae. Finally, one has the sum of two hypergeometric functions instead of one.

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