Oscillation of the photoabsorption near the ionization threshold for hydrogen-like atoms in electric and magnetic fields

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The cross section for the photoabsorption by atoms in weak electric and magnetic fields near the ionization threshold is found to contain some oscillating components associated with the unstable periodic paths. These components are expressed in terms of the parameters of the periodic paths. The results are in good agreement with the experimental data.

1. Recent experiments on laser photoexcitation of hydrogen atoms placed in a magnetic field[1,2] and electric field[3,4] have confirmed the data of previous experiments on the existence of regular oscillations near (and above) the ionization threshold of a free atom. Although the strengths of the external fields (expressed in atomic units) are small in the experiments that were carried out, this small value disappears in the case of the transitions to the highly excited states, which complicates the use of approximate methods and makes it necessary to seek a direct numerical solution of the relevant equations (see Refs. 3, 5, and 6 and the bibliographics cited there).

In the present letter we show that simple semiclassical equations for the absorption of a photon by atoms in external fields can be obtained and that the role of Planck's constant is played by a power of the external field.

2. The principal result of this study can be summarized as follows. The photoabsorption cross section near the ionization threshold can be represented in the form

$$\sigma(E) = \sigma_C + \beta^{1/6}\,\mathrm{Im}\sum_p \sigma_p^{(m)} \exp\left(i\frac{S_p}{\beta^{1/3}}\right) \tag{1}$$

for an external static magnetic field and it can be represented in the form

$$\sigma(E) = \sigma_C + \gamma^{1/4}\,\mathrm{Im}\sum_p \sigma_p^{(e)} \exp\left(i\frac{S_p}{\gamma^{1/4}}\right) \tag{2}$$

for an external static electric field. In these equations $\beta = B/(4.7\times10^5\ \mathrm{T})$ and $\gamma = F/(5.1\times10^9\ \mathrm{W/cm})$ are the magnetic and electric field strengths, expressed in atomic units (for a hydrogen atom), and σ_C is the cross section of a purely Coulombic photoabsorption. The sum in Eqs. (1) and (2) is taken over all unstable periodic paths which go through the Coulomb center, S_p is the reduced action along a given path, and $\sigma_p^{(m)}$ and σ_p^e are the amplitudes expressed in terms of the elements of the monodromy matrix of the periodic path under consideration and in terms of the wave function of the initial state.

3. Let

$$A_{\mathbf{p}} = |\mathbf{p}|^{1/2} \int (\psi_{\mathbf{p}}^{(-)}(x))^* \, \mathbf{e} \vec{\nabla} \psi_0(x) d^3x , \tag{3}$$

where $\psi_{\mathbf{p}}^{(-)}(x)$ is a standard solution of the Schrödinger equation in a Coulomb attractive field which behaves asymptotically as a plane wave (with a single coefficient) plus a converging spherical wave (see, e.g., Ref. 7), $\psi_0(x)$ is a wave function of the initial state, and $\mathbf{e}$ is a polarization vector of an incident photon. We can show that

$$\sigma_C = \frac{\alpha}{2\pi\omega} \int |A_{\mathbf{p}}|^2 \, do_{\mathbf{p}} , \tag{4}$$

$$\sigma_p^{(m)} = \frac{(8\pi)^{1/2}}{\omega} \alpha (\sin(\theta_1)\sin(\theta_2))^{1/2} A_{\mathbf{p}_1}^* A_{-\mathbf{p}_2} \times \frac{1}{|M_{12}|^{1/2}} \exp\left(-i\frac{\pi}{2}\nu + i\frac{\pi}{4}\right), \tag{5}$$

$$\sigma_p^{(e)} = \frac{2\alpha}{\omega} A_{\mathbf{p}_0}^* A_{-\mathbf{p}_0} \frac{1}{|M_{12}|} \exp\left(-i\frac{\pi}{2}\nu\right) , \tag{6}$$

where α is a fine structure constant, and ω is the photon frequency. For an atom in a magnetic field there is an infinite number of periodic paths, each of which emerges from the center with a momentum $\mathbf{p}_1$ at an angle θ_1 with respect to the z axis (running along the direction of the field) and returns to the center with a momentum $\mathbf{p}_2$ at an angle θ_2 (see, e.g., Refs. 1, 2, and 5). These initial and final angles and momenta are taken into account in Eq. (5).

In the case of an atom in an electric field at $E>0$ there is only one unstable periodic path which emerges from the center, running along the z axis in the direction opposite to the field, and which is reflected back to the center. Accordingly, $\sigma_p^{(e)}$ in (6) depends exclusively on $\mathbf{p}_0$, the momentum directed along the z axis. The coefficient of the exponential function in (5) and (6) is expressed in terms of M_{12}—the element of the monodromy matrix of the linearized equations—which relates the deviations in the plane perpendicular to the path to the deviations in the velocity at the starting point and end point. Let y be the deviation from the path in parabolic coordinates: $\mu^2 = r+z$, $\nu^2 = r-z$. The monodromy matrix in (5) and (6) can be determined from the relations

$$\begin{pmatrix} y_f \\ \dot{y}_f \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} y_i \\ \dot{y}_i \end{pmatrix} . \tag{7}$$

The quantity ν in (5) and (6) is an integer which is related to the additional phase shift near the points at which the semiclassical approximation breaks down:

$$\nu = \nu_0 + \nu_1 + 2m\nu_2 + 2\nu_3 , \tag{8}$$

where ν_0 is the number of conjugate points along the path (at which $M_{12}=0$), ν_1 is

the number of reflections from the boundaries, ν_2 is the number of reflections from the $\rho = 0$ axis, ν_3 is the number of times the path goes through the center, and m is the azimuthal quantum number of the final state. For states with small values of m, S_p and M_{12} can be assumed to be independent of m.

4. The expressions presented above were obtained by a method similar to that used in Refs. 8 and 9 for the construction of highly excited wave functions of an ergodic stadium billiard system. This system is based on the semiclassical Green's function in the Schrödinger equation in an external field, expressed as a sum over all classical paths that connect two fixed points (see, e.g., Ref. 10). In this problem the Coulomb singularity modifies slightly the standard expressions, which accounts for the appearance of the Coulomb functions $\psi_p^{(-)}$ in (5) and (6).

5. Here are several examples of the way in which these equations can be used. For a hydrogen atom in an electric field the cross section for the absorption of a photon, with the polarization parallel to the field, from the initial state with parabolic quantum numbers $n_1 = 1$, $n_2 = 0$, and $m = 0$ has the form

$$\sigma(E) = \sigma_C \left(1 + g\gamma^{1/4} \sum_{n=1}^{\infty} \frac{\lambda}{\sinh(\lambda Tn)} \sin\left(\frac{S}{\gamma^{1/4}} n + \pi n\right)\right), \tag{9}$$

where

$$\sigma_C = \frac{43 \times 2^{13} \pi^2 e^{-8}}{15} \approx 0.568; \quad g = \frac{3 \times 5^3}{43} \approx 8{,}72; \quad \lambda^2 = 2e; \quad e = E/\gamma^{1/2};$$

$$S(e) = \oint (4 + 2e\mu^2 - \mu^4)^{1/2} \, d\mu \approx 4.94 + 1.69e + 0.463e^2$$

$$T(e) = \oint \frac{d\mu}{(4 + 2e\mu^2 - \mu^4)^{1/2}} \approx 1.85 + 0.21\, e - 0.06\, e^2 \, .$$

In the initial state with the quantum numbers $n_1 = 0$, $n_2 = 1$, and $m = 0$ the oscillating term is twenty-five times smaller. These results are in very good agreement with the experimental data of Ref. 3 and with a straightforward numerical solution of the Schrödinger equation.[3]

For atoms in a magnetic field the situation is more complicated. In this case there is an infinite number of unstable periodic paths, and a closed expression such as (9) cannot be obtained. By averaging the cross section over a small interval ΔE (which is equivalent to measuring the cross section with a finite resolution) we see that the principal contribution to sum (1) comes from a small number of paths, the travel time along which is limited by the inequality[8,9]

$$T \leqslant 2\pi\beta^{3/4} / \Delta E \, . \tag{10}$$

The necessary parameters of such paths can easily be found numerically. The calculated contribution to the cross section for the absorption of a photon with a polarization parallel to the field for a hydrogen atom in the $2p$ state with $m = 0$, which corresponds to a very simple path directed along the z axis, is

$$\sigma(E) = \sigma_C \left(1 + g\beta^{1/6} \sum_{n=1}^{\infty} \frac{1}{|M_{12}|^{1/2}} \left(\frac{\sinh(\lambda)}{\sinh(\lambda n)}\right)^{1/2} \sin\left(\frac{Sn}{\beta^{1/3}} - \frac{3\pi}{2}n + \frac{\pi}{4}\right)\right), \tag{11}$$

where

$$\sigma_C = \frac{69 \times 2^{14}\pi^2 e^{-8}}{45} \approx 0.607; \quad g = \frac{45\ (2\pi)^{1/2}}{69} \approx 1.635; \quad e = E/\beta^{2/3};$$

$$S(e) = 2\oint (2 + 2e\mu^2 - \mu^6)^{1/2} d\mu \approx 5.783 + 2.094\, e + 3.014\, e^2;$$

$$|M_{12}(e)| \approx 2.82 + 3.61\, e + 1.25 e^2; \quad \lambda^2(e) \approx 1.73 + 8.5\, e - 0.14 e^2.$$

The contributions of some of the other paths can easily be calculated. These results are in good agreement with the experimental data[1,2] and with the numerical solution of the Schrödinger equation.[5]

6. All the calculations, taken collectively, show that the formalism of the unstable periodic paths[8,9] describes adequately the observed oscillations of the photoabsorption by atoms in external fields. The method which was used can be applied to a broad range of problems (both integrable and nonintegrable), in which there are unstable periodic paths, action along which is considerable.

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