Fast elastic e-H($2s$) scattering in laser fields

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A numerical method for the evaluation of the Born–Floquet amplitude for laser-assisted scattering is proposed for the case when a large basis set is required to achieve convergence. The method is applied to analyze the elastic scattering of fast electrons by the H($2s$) state in a low-intensity laser field of varying frequency and to study the resonant scattering with increasing laser intensity. While the behavior of an atom in a resonant field of low intensity is determined by virtual transitions between resonant levels, at high intensity a great number of nonresonant virtual transitions may significantly influence laser-assisted processes. As a consequence, the attenuation of resonant effects could appear, as well as the ''local'' stabilization of the atom against ionization. [S1050-2947(97)00411-3]

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I. INTRODUCTION

Laser-assisted processes involving excited atoms and collisions of electrons with these excited atoms are of interest for the understanding of processes in plasma heating by an intense electromagnetic field, gas breakdown, etc. Due to the larger spatial extension of excited atoms and to the closer coupling with other excited states, the dynamics of these processes can differ significantly from those involving ground-state atoms [1]. The excited species are also of particular importance in studies of high-intensity laser-assisted phenomena since the same physical effects would appear at much lower intensities if the initial state is chosen to be an excited state, for then the internal Coulomb field scales as n^{-4}, where n is the principal quantum number of the initial state. This is the reason why considerable effort has been devoted in recent years to the study of the phenomenon of strong-field suppression of ionization in the initially prepared excited circular and noncircular states, both experimentally [2] and theoretically [3,4].

The purpose of this paper is to study the elastic scattering of fast electrons ($E_i = 500$ eV) by hydrogen in the $2s$ state, in the presence of a linearly polarized laser field. Apart from an analysis of scattering in low-intensity fields of various frequencies, we will pay particular attention to the investigation of the intensity dependence of resonant scattering and in particular high-intensity scattering, where the initial $2s$ state is, by multiphoton transitions, directly or indirectly strongly coupled with Rydberg states.

II. METHOD

We have applied the nonperturbative Born–Floquet theory with a complex Sturmian basis-set expansion method [5]. During the collision a *net* number N of photons are transferred between the electron-atom system and the field. The geometry in which the polarization vector of the field is oriented along the momentum transfer **K** is adopted. Apart from some inconvenience in experimental measurements [6], this geometry has the advantage of giving the maximal coupling between the colliding system and the field when the momentum transfer is small [7].

Since the Born–Floquet theory is developed and discussed in detail in Ref. [5], we will give here only a brief outline. The present numerical method is proposed for calculating the scattering amplitude in the cases where the initial state is strongly coupled with higher excited states, which involve an expansion over a large basis set.

Let us consider a collision in a classical, spatially homogeneous, linearly polarized, monochromatic, and single-mode electric field. The nonrelativistic incident electron moving in that field is described by a Volkov wave function [8], which represents the exact solution of the time-dependent Schrödinger equation in the dipole approximation. The interaction between the laser field and the atom is treated nonperturbatively too by applying the Floquet method [9]. Finally, the interaction of the fast incident electron and the atom is treated by the first Born approximation. The calculation is performed by expanding the wave functions of the target atom dressed by the field on a discrete basis of complex Sturmian functions, which allows us to take exactly into account the bound- and continuum-state contributions in the dressing of the target atom. This feature of the Sturmian expansion is of crucial importance for electron collisions with excited states of atoms, where many states are coupled with the initial one, including high Rydberg states and the continuum. The Sturmian functions are given by

$$S_{nl}^{\kappa}(r) = N_{nl}^{\kappa}(2\kappa)^{l} r^{l+1} e^{-\kappa r} L_{n-l-1}^{2l+1}(2\kappa r), \tag{1}$$

where N_{nl}^{κ} is a normalization constant, $L_n^{\alpha}(x)$ are the associated Laguerre polynomials, and κ is a complex parameter. By choosing the ''wave number'' $\kappa_s = -i\kappa$ to lie in the upper right quadrant, one can implement implicitly the Siegert boundary conditions, i.e., those of the atom decaying in a laser field [9]. In the time-independent Floquet formalism these boundary conditions have the consequence of giving complex quasienergies

$$E = E_i + \delta_i - i\Gamma_i/2, \tag{2}$$

where δ_i is the shift from the unperturbed energy E_i and Γ_i is the induced width.

The first Born–Floquet scattering amplitude for the elastic scattering accompanied by the transfer of N photons is given by

$$f^{B1,F}_{f,i,N}=e^{-iN\phi}\sum_{M,M'=-\infty}^{+\infty} i^{M-M'}J_{N+M'-M}(\mathbf{K}\cdot\boldsymbol{\alpha}_0) \times\sum_{n'l'}\sum_{nl} c^{M'}_{n'l'}c^{M}_{nl}\, f^{B1}_{n'l'm_i,nlm_i}, \tag{3}$$

where $\mathbf{K}=\mathbf{k}_i-\mathbf{k}_f$ is the momentum transfer in the collision, J_l is the Bessel function, and c^M_{nl} are coefficients of expansion of the radial part of Floquet harmonic components $\mathcal{F}_M(\mathbf{r})$ on the Sturmian basis functions $S^{\kappa}_{nl}(r)$. $\mathcal{F}_M(\mathbf{r})$ represents the electron that has exchanged a total of M photons with the laser field, both real and virtual. The amplitude $f^{B1}_{n'l'm_i,nlm_i}$ is given by the expression

$$f^{B1}_{n'l'm_i,nlm_i}=\frac{-2}{K^2}\int d\mathbf{r}\; r^{-2}S^{\kappa}_{n'l'}(r)Y^{*}_{l'm_i}(\hat{\mathbf{r}}) \times[e^{i\mathbf{K}\cdot\mathbf{r}}-1]S^{\kappa}_{nl}(r)Y^{*}_{lm_i}(\hat{\mathbf{r}}). \tag{4}$$

The angular part of the integral (4) is performed by expanding the plane wave $e^{i\mathbf{K}\cdot\mathbf{r}}$ in partial waves. This gives rise to radial integrals of the form

$$R^{\lambda}_{n'l',nl}=\int_0^{\infty} dr\; S^{\kappa}_{n'l'}(r)j_{\lambda}(Kr)S^{\kappa}_{nl}(r). \tag{5}$$

The integral (5) has the same form as the radial part of collisional form factors [10]. An analytical evaluation of this integral is not readily obtainable, and in the general case the result is expressed in terms of generalized hypergeometric functions. The hypergeometric function represents essentially a factorial series, and for large values of the parameters n or n' it produces a considerable loss of precision. This arises mainly from the rounding error in the summation of the series in which successive terms can vary by two or three orders of magnitude. However, if a relatively small basis set (with a basis state number $n<30$ and angular basis states $l<7$) is required for convergence, which is usually fulfilled for a low-intensity laser field, one can expand the spherical Bessel function either in a power series in Kr, when the momentum transfer is small, or in a power series in $(Kr)^{-1}$. In both cases, one is left with the following integrals to compute:

$$I(n,m)=\int_0^{\infty} dr\; L^{\alpha}_n(cr)r^{\delta}e^{(c+s)r}L^{\gamma}_m(cr), \quad \mathrm{Re}(c+s)>0. \tag{6}$$

In the earlier papers [5,7,11] we have generated these integrals by using the following recurrence relation between them [11]:

$$I(n+1,m)=\frac{c}{(c+s)(n+1)}\left[\left(\frac{s}{c}(2n+\alpha+1)+(n+\alpha-m-\delta)\right)I(n,m)-\frac{s}{c}(n+\alpha)I(n-1,m)+(m+\gamma)I(n,m-1)\right]. \tag{7}$$

However, with the increase of laser intensity many states of the atom become coupled, including high Rydberg states and the continuum. In this situation a large basis set is necessary to achieve converged results. For high values of n, l, n', l', the recurrence relation (7) produces a loss of precision due to the rounding error in the summation of the two terms on its right-hand side. We have found that the best method to calculate the scattering amplitude (3) involving high values of n,l and n', l' is not to calculate separately the integral (5) and after that to perform the summation over n,l and n',l', but rather to perform first the summation over the indices n,n', before resolving numerically the resulting integral over radial variable r, and finally to sum over l,l'. Thus we have first generated the values of the associated Laguerre polynomials for a given mesh of the points of the radial variable r by using the upward recurrence relation [12]. This recurrence relation is found to be stable for values of n up to 90 and for small values of r up to values of r equal to several thousand atomic units. Then the summation over n, of the quantities $c^M_{nl}S^{\kappa}_{nl}(r)$, is performed. Finally, the resulting radial integration is performed by employing a Gaussian quadrature scheme. To test the present method we have, among other calculations, obtained agreement with the those previously reported in [5]. The spherical Bessel function appearing in Eq. (3) is evaluated by Steed's method [13].

We note that the order of summation and the integration in Eq. (3) would not be of importance if the radial integral (5) can be expressed in closed form instead of being reduced to the summation of a slowly converging or factorial series. In fact, it has been shown that the radial parts of the collisional form factors can be expressed in terms of the integer order Bessel functions, under the condition that $l,l'\ll n,n'$ and $\max(\Delta n,\Delta n')\ll n,n'$ [10].

III. RESULTS AND DISCUSSION

The cross sections for the elastic electron-atom scattering with no photon transfer in a field of moderate intensity are almost indistinguishable from the field-free cross section under the same kinematic conditions. For that reason, in Fig. 1 we show only the differential cross sections as a function of scattering angle θ, corresponding to the exchange of $N=-1$ photons by the laser field of the same intensity $I=1.327\times10^9$ W/cm^2, but various frequencies: $\omega=4.95$ eV (Kr*F excimer laser), $\omega=2.0$ eV (He:Ne), $\omega=1.165$ eV (Nd:YAG where YAG denotes yttrium aluminum garnet), and its first harmonic $\omega=2.33$ eV and $\omega=0.827$ eV.

The forward differential cross sections rise with decreasing frequency; one can explain this feature by the augmentation of the mean size of the atom, whose amplitude of quiver oscillations changes by a factor proportional to $\alpha_0=\sqrt{I}/\omega^2$, which increases the probability of scattering at large impact parameters. However, the probability of forward scattering is not a monotonically increasing function of $1/\omega$ if ω is comparable to any characteristic excitation fre-

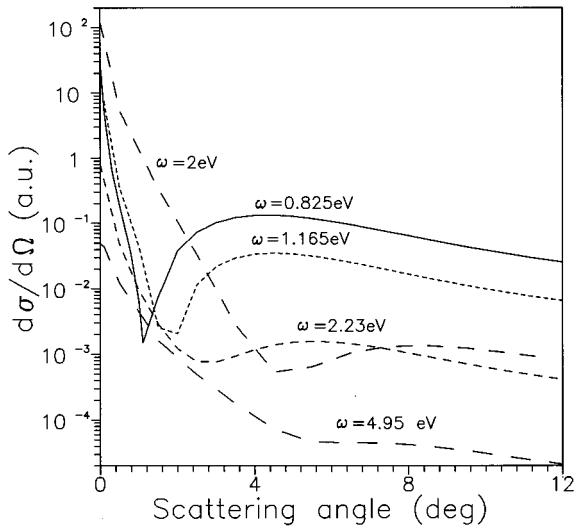

FIG. 1. Differential cross section (in a.u.) for the elastic electron scattering on hydrogen in the $2s$ state in the presence of a linearly polarized laser field (parallel to the momentum transfer) of various frequencies ω and intensity $I=1.327\times10^{9}$ W/cm^2, as a function of the scattering angle θ (in degrees). The incident electron energy is $E_i=500$ eV. N is the *net* number of photons exchanged by the e-H system and the field in the collision.

quency of the atom. Thus the He:Ne laser resonantly couples the $2s$ state with the $3p$ state even at low intensities, with a detuning of $\delta\omega=0.1$ eV at $I=1.327\times10^{9}$ W/cm^2. The same states are also strongly coupled by the field of the YAG laser. The (nearly) resonant collisions in these fields are governed by the virtual process of excitation of the H atom, by the projectile, to the $3p$ state, and its successive deexcitation to the $2s$ state, by the stimulated emission of a photon. Away from the resonance, the inverse process with the emission of a photon in the initial state also becomes important. The constructive interference of the two virtual processes causes the peak of the differential cross sections in the forward direction, it being highest in the resonant case. On the other hand, the minimum in the cross section, appearing at a relatively small scattering angle, is a consequence of the destructive interferences between the process of no photon absorption and the above-mentioned virtual processes. With the exception of $\omega=2$ eV, the position of the minimum shifts toward a larger scattering angle and almost disappears with increasing frequency. We note that under the same conditions, the elastic cross sections for the inverse and stimulated bremsstrahlung of the same number of photons are very close in the whole range of frequencies considered here.

As the second example we show in Fig. 2 the differential cross sections for elastic electron scattering by the H($2s$) state in the three distinct cases of a relatively low-, moderate-, and high-intensity field with the values $I_1=1.327\times10^{9}$ W/cm^2, $I_2=10^{11}$ W/cm^2, and $I_3=10^{13}$ W/cm^2, respectively, in the vicinity of the one-photon $2s$-$3p$ resonance. The $2s$-$3p$ resonant coupling governs the e-H scattering involving the $n=2$ or 3 level as either the initial or final state, in the field of the YAG, He:Ne, and not very different frequency lasers of low and moderate intensity [7].

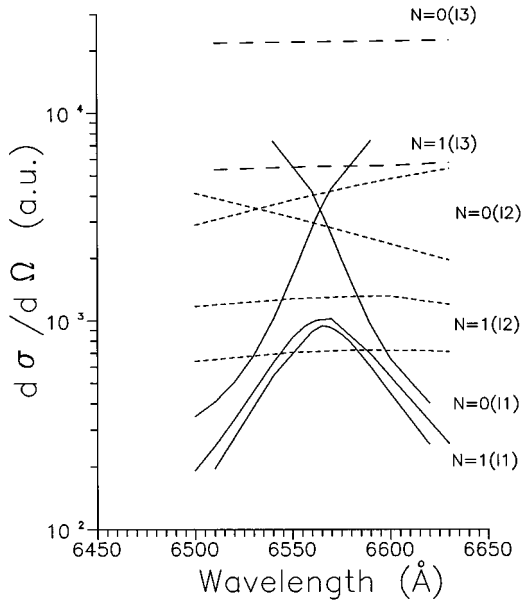

FIG. 2. Differential cross sections for the elastic e-H($2s$) scattering, in the vicinity of a one-photon $2s$-$3p$ resonance, at $\theta=0.5°$, versus wavelength (in angstroms). Solid line, cross sections corresponding to the intensity $I_1=1.327\times10^{9}$ W/cm^2; dotted line, cross sections corresponding to the intensity $I_2=10^{11}$ W/cm^2; dashed line, cross sections corresponding to the intensity $I_3=10^{13}$ W/cm^2.

At low intensity I_1, the real adiabatic quasienergy curves $2s$ and $3p$ are very distorted by the mutual coupling in a narrow region of wavelengths, where they exhibit an avoided crossing close to the wavelength 6566 Å. The coupling of the resonant levels by the rest of the spectrum is negligible. The character interchange of the two resonant levels at a resonant wavelength manifests clearly in the $N=0$ cross sections for the elastic electron scattering by the $2s$ and $3p$ states evolving adiabatically with laser frequency. On the other hand, if one considers collisions by the diabatic quasienergy levels along which the initial character of the state is preserved, one can see that the cross sections show pronounced extrema in the resonant region. This is a consequence of the increasing contribution of the virtual process in which the atom by resonant absorption of a photon passes to the $3p$ state and then deexcites either by the collision with the projectile (this is the dominant process for the $N=1$ amplitude) or by a stimulated emission of a photon, with the intermediate elastic scattering with the projectile (the dominant process for the $N=0$ scattering amplitude). Far from resonance, the elastic scattering of the dressed projectile with the static potential of the nondressed H($2s$) state is the dominant process. In other words, the e-H($2s$) scattering in a low-intensity field whose frequency brings the $2s$ state into resonance with a higher state may be regarded as a field-free electron scattering by a mixed state, which can be expressed by a linear superposition (with equal coefficients at the resonance) of the two unperturbed states to which the resonant ''dressed'' states reduce in the low-intensity limit. Since the ''mixed'' state

acquires larger spatial extension when one approaches the resonant frequency (due to an increasing contribution of the higher state), the small-angle elastic e-H($2s$) cross sections grow in the resonant region. Furthermore, at low intensity the $N=1$ cross sections for electron scattering from the adiabatic dressed $2s$ or $3p$ level are different only by a few percent in the resonant region. It is a consequence of the fact that the $2s$ and $3p$ Floquet wave functions are essentially similar superpositions of the same unperturbed states near resonance. The small differences in the cross sections are caused by respective constructive and destructive interferences of the above-mentioned dominant process for a particular collision and other virtual processes whose individual contributions are rather small.

As the intensity increases (I_2), the coupling between resonant levels (which is proportional to their separation at the point of the closest approach) increases, as well as the coupling of a resonant level by the rest of the spectrum (the measure of this coupling is given by the induced width Γ_i). The slopes of the real quasienergy curves $2s$ and $3p$ are smaller in the resonant region than at low intensity, due to larger influence of higher nonresonant states. The cross sections show a similar behavior. While the crossing of the $2s$ and $3p$ adiabatic quasienergy levels shifts towards larger wavelength with increasing intensity, the $N=0$ cross sections for electron collisions with an atom in these levels intersect by small angle at lower wavelength (for several tens of angstroms), owing to the interference effects. The separation of the $N=1$ cross sections enlarges with intensity due to the simultaneous increasing contribution of higher-order processes and decreasing contribution of the dominant one and their interferences that keep the same trend as at low intensities.

At the highest intensity (I_3) there is no avoided crossing between the $2s$ and $3p$ levels and no structure in the cross sections is observed in a wide region of wavelengths. Although the successive one-photon inverse and stimulated bremsstrahlung is still the process with the largest contribution, the virtual processes involving bremsstrahlung with up to four photons give individual contributions to the scattering amplitude greater than 1%. It is obvious that in a strong field the dominant type of coupling is the Raman coupling with the high Rydberg levels and the low continuum. The physical consequence of this type of coupling is a formation of a spatially extended wave packet that manifests itself in e-H collisions by large forward differential cross sections.

The electron collision with the H($2s$) state of hydrogen in the field of a YAG laser of intensity greater than 2×10^9 W/cm^2 is influenced by the strong three-photon resonant coupling of the $2s$ state with a high Rydberg level [9]. The quasienergy curves of these two levels exhibit an avoided crossing not far below the multiphoton ionization threshold of $2s$ state at about $I=7\times10^{11}$ W/cm^2. The calculation is difficult to handle in the vicinity of this resonance because of the large spatial extension of the atomic wave function, which, being a linear superposition of the $2s$ and Rydberg wave function, may range up to several thousand atomic units. The additional complication arises from the high oscillatory character of the low-angular-momentum resonant Rydberg level (with $l\leqslant3$), which requires a large number of the mesh points in the numerical integration. Further, the

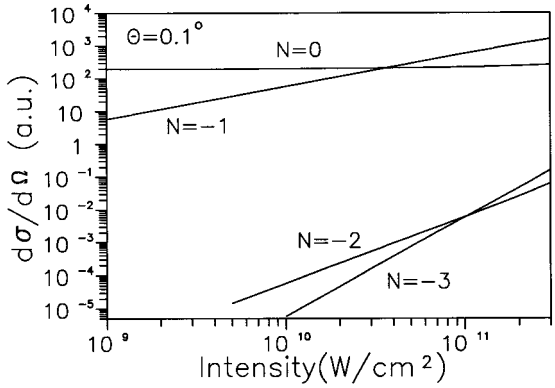

FIG. 3. Differential cross sections for the elastic e-H($2s$) scattering, in the field of a Nd:YAG laser of a varying intensity, at a scattering angle $\theta=0.1°$.

convergence of the scattering amplitude (3) and (4) expanded on a Sturmian basis depends crucially on the ''wave number'' κ_s, a parameter that adjusts the tail of the exponentially decreasing Sturmian functions. In the present case the choice of this parameter is delicate because of the obvious inability of the basis set to represent both the $2s$ and the highly excited states with sufficient accuracy. Our intention is to study the influence of high excited states on the scattering process, which is one of the greatest challenges in atomic collision activities today. The present example gives us a good opportunity to do this by analyzing the forward scattering, where the largest contribution comes from the states with broad spatial extension. Of course, it is necessary to represent adequately the highly excited states in the basis. The choice of the parameter κ_s, which has a small real part, satisfies this requirement since it produces a long tail of the Sturmian functions. In the present example we have used $\epsilon_s=\kappa_s^2/2=-0.05$ a.u. and $\theta_{k_s}=10°$. The basis set presently employed consists of harmonic components with photon index between -7 and 13, each of these components being expanded on a basis of 80 (or 90) complex Sturmian functions for each value of l $(0\leqslant l\leqslant7)$ that is used. The integration is carried out over the radial variable by a Gaussian quadrature scheme, up to 400 a.u. or 1000 a.u. (so that the grid spacing is set to about $1a_0$ in the most unfavorable case). We have been able to obtain convergent cross sections up to the intensity 3×10^{11} W/cm^2. Our results for the nearly forward differential cross sections are presented in Fig. 3. The cross sections show a rapid increase with intensity, being faster for larger N. This is a consequence of both the three-photon resonant transitions and other higher-order processes that are more important for scattering with $|N|>1$. Away from the resonant intensity, the dominant contribution to the scattering amplitude comes from the virtual processes in which the atom first passes to a high Rydberg state lying in a band $\pm\hbar\omega$ around the resonant level and subsequently collides with the dressed projectile, which leads to the redistribution of population of atomic electrons. Finally, by the process of stimulated bremsstrahlung it is deexcited from the band $\pm\hbar\omega$ to the $2s$ state. In the vicinity of the resonant intensity, the three-photon resonant transitions govern the scattering. Among them, those ending in the Rydberg state

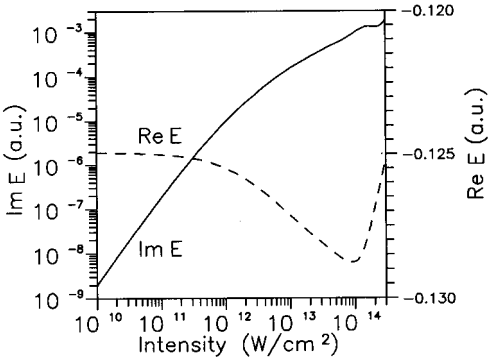

FIG. 4. Real (dashed line) and imaginary (solid line) parts of the energy eigenvalue of the $2s$ state vs intensity, for hydrogen irradiated by linearly polarized light of frequency $\omega=2.8$ eV.

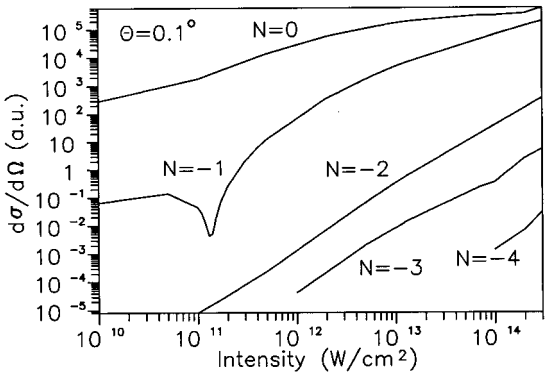

FIG. 5. Differential cross sections for the elastic e-H($2s$) scattering, in the field of a varying intensity and a frequency of 2.8 eV, at a fixed scattering angle $\theta=0.1°$.

with angular momentum $l=3$ give the dominant contribution to the scattering amplitude. This leads to the conclusion that the Rydberg state that is resonant with the $2s$ state is one that has f symmetry. We have not been able to extract from our results more information about the state. Anyway, having in mind the impossibility to calculate precisely the eigenvalue of a state just below a multiphoton ionization threshold, because an infinite number of Rydberg states accumulate there, and other limitations in our calculations, we may consider our analysis rather qualitative.

Finally, we have made an investigation of e-H($2s$) elastic scattering in a field whose frequency $\omega=2.8$ eV almost tunes the $2s$ state into resonance with the $5p$ state in the low-intensity limit. This is an interesting example to investigate because a substantial suppression of ionization has been observed for the H atom exposed to both short and relatively long laser pulses of peak intensities of order 10^{13} W/cm^2. The question is whether the same physical effects are observable for stationary pulses under similar conditions, which is implemented implicitly in the Floquet description of an atom in a laser field [14]. In order to answer this question we have studied the eigenenergy curve of the $2s$ state as a function of the laser intensity, as shown in Fig. 4. At intensities above 10^{12} W/cm^2, the one-photon coupling of the $2s$ state with superposition of the $5p$ and $5f$ states, which are degenerate in the low-intensity limit, becomes increasingly important. This coupling achieves its maximum value at about 8×10^{13} W/cm^2, but no crossing of the eigenenergy curves is found. In addition to a (nearly) resonant transition between the two levels, at high intensities a number of nonresonant virtual transitions could influence the total effect in a laser-assisted atomic process. Thus, at the intensity 8×10^{13} W/cm^2, the two-photon virtual transitions to higher- and lower-energy spectra give a contribution that contributes almost 10% to the norm of the Floquet wave function. A similar conclusion follows from the investigation of forward elastic e-H($2s$) differential cross sections. The contribution from two-photon and higher-order processes increases rapidly with the intensity. Since the Floquet wave function can be viewed as a linear superposition of states of the entire spectrum, it is obvious that the spatial distribution of the atomic wave function is less compact at higher intensities than at those where a strong coupling between the $2s$ state and $5p/5f$ states is dominant. Thus, in addition to the central part of the atomic wave packet, which is located between the mean radii of the $2s$ and $5p/5f$ states, it has also a part that is far from the nucleus, where it is unlikely that it can absorb a photon, and another one closer to the nucleus, which is more strongly bound and thus requires more photons to be ionized. This ''spreading'' of the atomic electron distribution provides more stability against ionization. Indeed, one can observe a plateau and a region where the imaginary part of the $2s$ state is seen to decrease, for intensities in the region between 8×10^{13} and 2.2×10^{14} W/cm^2. Of course, with the increase of intensity, the coupling with the continuum becomes more important and causes the increase of photoionization yield.

The forward differential cross sections, shown in Fig. 5, are increasingly peaked in the forward direction with increasing intensity, with a somewhat slower rate of increase of the $N=0$ cross section in the region of ''stabilization.'' This rapid rise is an indirect manifestation of the fact that the electron collides with a spatially very large and growing wave packet with increasing intensity. At the highest intensities considered here, the largest basis set that was necessary in order to obtain convergence consists of harmonic components with photon indices ranging from -7 to 19, together with the radial Sturmian basis with indices $l_{\max}=19$ and $n=50$. The destructive interferences cause the minimum in the $N=-1$ cross section.

In conclusion, we have observed a region of local suppression of ionization, around 10^{14} W/cm^2 in intensity, in a field of 4428 Å wavelength. It is located on the higher-intensity side of the resonant intensity, where the $2s$ and $5p/5f$ states have the maximum coupling. This phenomenon is a consequence of the redistribution of the population from the $2s$ state to higher- and lower-energy states rather than predominantly to the $n=5$ states as is the case under fully resonant conditions, which results in a smaller ionization rate.

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