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Static-Electric-Field-Induced, High-Energy Plateau for Scattered X-Ray Photons in Laser-Assisted, X-Ray–Atom Scattering

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We consider scattering of x rays by H atoms in the presence of both a linearly polarized laser field and a static electric field. Results for the differential cross section as a function of the number of photons n exchanged with the laser field are presented. For x-ray–atom scattering in the presence of a 10^{14} W/cm² laser field the differential cross section has a plateau only for emitted photons ($n < 0$). Adding a static electric field gives rise to an extended plateau for absorbed photons ($n > 0$), indicating a substantial increase of the scattered x-ray energies. We present a quasiclassical explanation of these results. [S0031-9007(98)07847-8]

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Laser-field induced or assisted atomic processes have attracted much interest in recent years [1,2]. Using strong laser fields, it is possible to generate harmonic photons with an energy of almost 500 eV [3]. Coherent x-ray sources with energies in the “water window” [between the K shell absorption edges of C (284 eV) and O (532 eV)] would have important applications to imaging living biological structures by means of x-ray holography [4]. However, the efficiency of generation of such high-energy photons is low. We propose here a means of obtaining such high-energy photons by laser-assisted, soft x-ray–atom scattering in the presence of a relatively weak static electric field (i.e., having a field strength of only a few percent of that of the laser electric field). X-ray–atom scattering in the presence of a laser field was recently considered theoretically [5]. Plateaulike structures in the differential cross section (DCS) as a function of the number of photons exchanged with the laser field were observed, but primarily for scattered x-rays having lower energy. It was also recently shown that the presence of a static electric field modifies the intensities of harmonics generated in a laser field [6]. We present here the theory of laser-assisted, x-ray–atom scattering in the presence of a static electric field. We show that for initial soft-x-ray photons having an energy of 50 eV, which may be obtained with high efficiency in the harmonic generation process [1,2], the energy of the scattered x rays may be increased by an order of magnitude.

A detailed derivation of the main expressions for the DCS for laser-assisted x-ray–atom scattering (including discussion of the approximations used) is presented in Ref. [5]. We therefore focus here on the effects of a static electric field. The DCS for laser-assisted x-ray–atom scattering with absorption ($n > 0$) or emission ($n < 0$) of n laser photons having frequency ω is [in SI plus atomic units ($e = \hbar = m = 1$)]

$$\frac{d\sigma(n)}{d\Omega_{\mathbf{K}'}} = c^{-4} \omega_{\mathbf{K}} \omega_{\mathbf{K}'}^3 |T_{\mathbf{K},\mathbf{K}'}^{(+)}(n) + T_{\mathbf{K}',\mathbf{K}}^{(-)}(n)|^2, \quad (1)$$

$$T_{\mathbf{K},\mathbf{K}'}^{(\pm)}(n) = \int_0^{2\pi} \frac{d\varphi}{2\pi} \mathcal{T}_{\mathbf{K},\mathbf{K}'}^{(\pm)}(\varphi) \exp(in\varphi).$$

Here $\omega_{\mathbf{K}}$ and $\omega_{\mathbf{K}'} = \omega_{\mathbf{K}} + n\omega$ are the energies of the incident and scattered x-ray photons, respectively. The T -matrix elements $T_{\mathbf{K},\mathbf{K}'}^{(\pm)}(n)$ are the Fourier components of the matrix elements [5]

$$\mathcal{T}_{\mathbf{K},\mathbf{K}'}^{(\pm)}(\varphi) = \int_0^\infty d\tau \int d\mathbf{q} \exp\{-i[S(\mathbf{q}; t, \tau) \pm \omega_{\mathbf{K}'}\tau]\} \\ \times \langle \psi_0 | \mathbf{r} \cdot \hat{\mathbf{e}}_{\mathbf{K}} | \mathbf{q} + \mathbf{A}(t) \rangle \langle \mathbf{q} + \mathbf{A}(t - \tau) | \mathbf{r} \cdot \hat{\mathbf{e}}_{\mathbf{K}'} | \psi_0 \rangle, \quad (2)$$

where $|\psi_0\rangle$ is the atomic ground-state ket vector, $|\mathbf{q}\rangle$ is a plane-wave ket vector for the electron, $\varphi \equiv \omega t$, and $\hat{\mathbf{e}}_{\mathbf{K}}$ and $\hat{\mathbf{e}}_{\mathbf{K}'}$ are the unit polarization vectors of the incident and scattered photons, respectively. $\mathbf{A}(t)$ and $S(\mathbf{q}; t, \tau) = \int_{t-\tau}^t dt' \{ \frac{1}{2} [\mathbf{q} + \mathbf{A}(t')]^2 + I_0 \}$, where $I_0 = 0.5$ a.u. is the ionization potential of the hydrogen atom, are, respectively, the vector potential and the electron’s quasiclassical action in the presence of both a laser field and a static electric field. The matrix element $T_{\mathbf{K}',\mathbf{K}}^{(-)}(n)$ corresponds to the process in which an x-ray photon having wave vector \mathbf{K} and energy $\omega_{\mathbf{K}}$ is absorbed first. The ionized electron propagates under the influence of both the laser and static electric fields during the time interval from $t - \tau$ to t , at which time it comes back to the atomic core (i.e., the return time is τ). The electron then recombines with the atomic core, exchanging n photons with the laser field and emitting an x-ray photon having wave vector \mathbf{K}' and energy $\omega_{\mathbf{K}'}$. The matrix element $T_{\mathbf{K},\mathbf{K}'}^{(+)}(n)$ describes the process in which the x-ray photon having wave vector \mathbf{K}' and energy $\omega_{\mathbf{K}'}$ is emitted first. Reference [5] shows that the contribution of $T_{\mathbf{K},\mathbf{K}'}^{(+)}(n)$ to the DCS can be neglected in comparison to the contribution of $T_{\mathbf{K}',\mathbf{K}}^{(-)}(n)$ (for $|n| > 5$). The three-dimensional integral over the intermediate electron momenta in Eq. (2) can be carried out using the time-dependent WKB approximation [5]. The integral over the return time τ is computed numerically, and, finally, the T matrices, which appear in Eq. (1), are obtained using the fast Fourier transform method.

The explicit analytical forms of the matrix elements in Eq. (2) are given in Ref. [5] in terms of the vector potential $\mathbf{A}(t)$, the stationary momentum $\mathbf{q}_s \equiv \mathbf{q}_s(t, \tau) = -\frac{1}{\tau} \int_{t-\tau}^t dt' \mathbf{A}(t')$, and the action $S_s \equiv S(\mathbf{q}_s; t, \tau)$. The vector potential $\mathbf{A}(t)$ corresponds to a linearly polarized electric field vector $\mathbf{E}(t) = (E_0 \sin \omega t + E_s) \hat{\mathbf{e}}$, where $\hat{\mathbf{e}}$ is the unit polarization vector. E_0 and E_s are the amplitudes of the laser and static electric field vectors, respectively. It follows that $\mathbf{A}(t) = -\int^t \mathbf{E}(t') dt' = (A_0 \cos \omega t - E_s t) \hat{\mathbf{e}}$ and $\boldsymbol{\alpha}(t) = \int^t dt' \mathbf{A}(t') = (\alpha_0 \sin \omega t - \frac{1}{2} E_s t^2) \hat{\mathbf{e}}$, where $A_0 = E_0/\omega$ and $\alpha_0 = A_0/\omega$. The stationary momentum can be written as $\mathbf{q}_s(t, \tau) = [\boldsymbol{\alpha}(t - \tau) - \boldsymbol{\alpha}(t)]/\tau$, while the stationary action is given by $S_s(t, \tau) = (I_0 + U_p)\tau - \frac{1}{2} \mathbf{q}_s^2 \tau + \mathcal{U}_1(\omega t) - \mathcal{U}_1(\omega(t - \tau))$, where $\mathcal{U}_1(\varphi) = U_p \sin 2\varphi/2\omega + [\frac{1}{6} E_s^2 \varphi^3 - E_s E_0 (\cos \varphi + \varphi \sin \varphi)]/\omega^3$, and $U_p = A_0^2/4$ is the ponderomotive potential of the laser field. One may easily verify that the functions $\mathbf{q}_s(t, \tau) + \mathbf{A}(t)$, $\mathbf{q}_s(t, \tau) + \mathbf{A}(t - \tau)$, and $S_s(t, \tau)$, which appear in the final result for $\mathcal{T}_{\mathbf{K}, \mathbf{K}'}^{(\pm)}(\varphi)$, are $2\pi/\omega$ -periodic functions of t , thereby justifying the use of Fourier expansion methods. This periodicity follows also from consideration of the Volkov Green's function for the case of both a laser field and a static electric field [7].

We present our numerical results for a laser field intensity $I = 10^{14}$ W/cm², and for different values of the static electric field strength. For simplicity, the polarization vectors of the incident and scattered x-ray photons are taken parallel to that of the linearly polarized laser field. The energy of the incident x rays is chosen to be $\omega_{\mathbf{K}} = 50$ eV. Figure 1 shows the DCS as a function of n for laser-assisted x-ray-hydrogen atom scattering in the absence (dashed curve) and presence (solid curve) of a

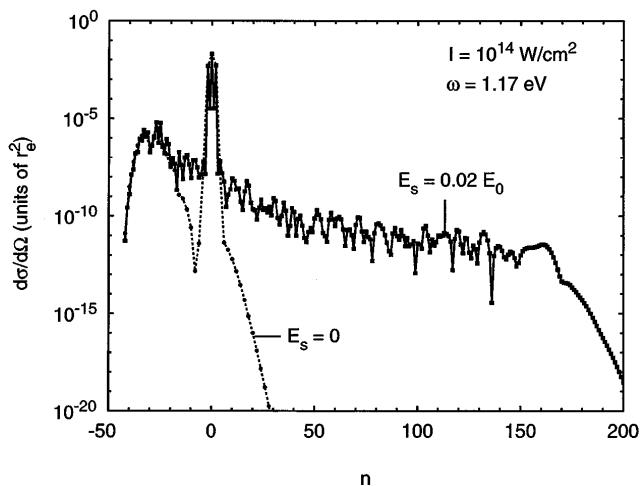


FIG. 1. The DCS for x-ray-hydrogen atom scattering in units of r_e^2 (where $r_e = 2.8 \times 10^{-15}$ m is the classical electron radius) as a function of the number of photons n exchanged with the laser field of frequency $\omega = 1.17$ eV and intensity 10^{14} W/cm² (dashed curve). The results including a static electric field $E_s = 0.02E_0$ are shown by a solid line. $\omega_{\mathbf{K}}$ for the incident x-ray photons is 50 eV.

static field having strength $E_s = 0.02E_0$ [8]. We note the following effects of the static electric field. First, the number of absorbed or emitted laser photons can now be not only even but also odd. Second, there is little effect on the DCS for either small values of $|n|$, for which there is a maximum, or negative values of n , for which there is a plateau. Third, for values of n between the plateau for negative n and the maximum for small $|n|$, the DCS is much larger. Fourth, and most significant, is the appearance of an extended plateau for positive values of n . The cutoff for this plateau is at $n = 162$, i.e., the energy of the scattered x rays is $\omega_{\mathbf{K}'} = 205\omega = 4.79\omega_{\mathbf{K}} = 240$ eV. Therefore, the addition of a static field having strength 2% of the laser electric field strength enables one to obtain scattered x-ray photons having energies up to almost 5 times higher than the incident energy.

In Fig. 2 we analyze how the plateau for positive n changes as a function of the ratio of the static and laser electric field strengths. As this ratio increases from zero

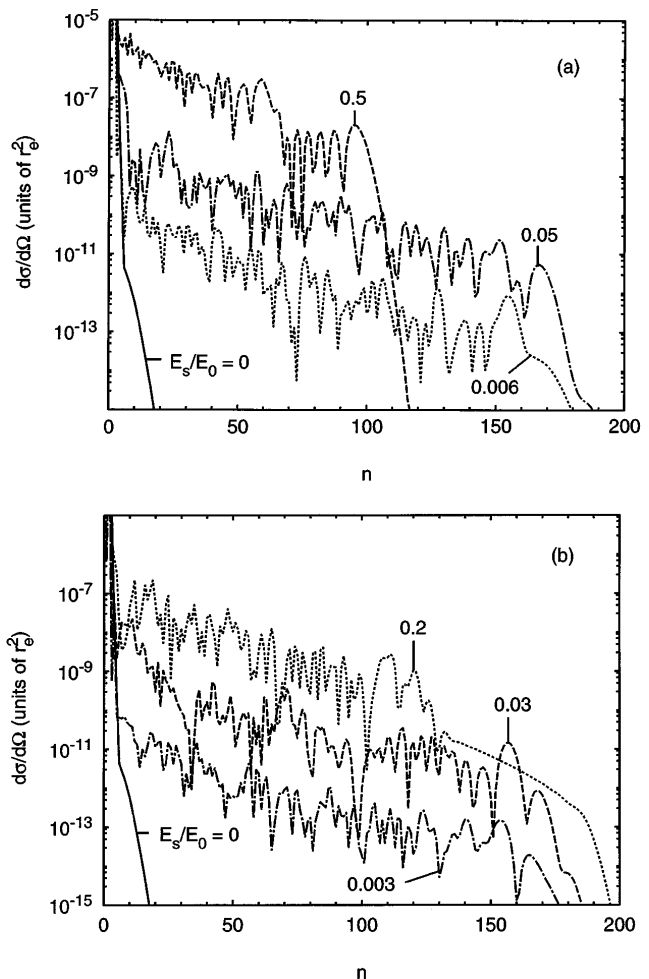


FIG. 2. The DCS for x-ray-hydrogen atom scattering as a function of the number of exchanged photons n for the same laser field parameters as in Fig. 1, but for different values of the static electric field strength (chosen in each figure to minimize overlap): (a) $E_s/E_0 = 0, 0.006, 0.05,$ and 0.5 ; (b) $E_s/E_0 = 0, 0.003, 0.03,$ and 0.2 .

to 0.05 the DCS increases, while the position of the cutoff is unchanged. As E_s/E_0 increases further, the position of the cutoff shifts to lower n and the DCS increases further. In the following we explain these results.

It was shown in Ref. [5] that a simple quasiclassical analysis of the x-ray spectra can be carried out by applying the saddle-point method to the integral over the return time τ in Eq. (2) and to the integral over $\varphi (= \omega t)$ in the matrix element $T_{\mathbf{k}, \mathbf{k}}^{(-)}(n)$ in Eq. (1). For the integral over τ , the saddle-point method implies the condition $\partial[S(\mathbf{q}; t, \tau) - \omega_{\mathbf{k}}\tau]/\partial\tau = 0$, giving $\frac{1}{2}[\mathbf{q} + \mathbf{A}(t - \tau)]^2 = \omega_{\mathbf{k}} - I_0$. According to this equation the atom is ionized by absorbing one x-ray photon of energy $\omega_{\mathbf{k}}$, and the electron is born at some time $t_0 = t - \tau$. The initial momentum of this electron is denoted by $\mathbf{p}_0 = p_0\hat{\mathbf{e}}$, where $p_0^2 = 2(\omega_{\mathbf{k}} - I_0)$. Assuming that $\mathbf{A}(t) = A(t)\hat{\mathbf{e}}$, $\alpha(t) = \alpha(t)\hat{\mathbf{e}}$, and $\mathbf{q} = \mathbf{q}_s(t_1, t_1 - t_0) = q_s\hat{\mathbf{e}}$, we obtain

$$\alpha(t_0) - \alpha(t_1) = [p_0 - A(t_0)](t_1 - t_0). \quad (3)$$

This equation is equivalent to the solution of the classical Newton's equation of motion of an electron in a laser field and a static electric field, under the condition that this electron is born at the nucleus, $\mathbf{r}(t_0) = \mathbf{0}$, with the initial momentum $\mathbf{p}_0 = p_0\hat{\mathbf{e}}$, and that at the time t_1 it returns to the nucleus, i.e., $\mathbf{r}(t_1) = \mathbf{0}$. The application of the saddle-point method to the integral over the time t implies that $\partial[S(\mathbf{q}; t, \tau) - n\omega t]/\partial t = 0$, so that we obtain the condition $\frac{1}{2}[\mathbf{q} + \mathbf{A}(t)]^2 - \frac{1}{2}[\mathbf{q} + \mathbf{A}(t - \tau)]^2 = n\omega$, from which it follows that the energy exchanged with the laser field at time t_1 is [with $\mathbf{q} \rightarrow \mathbf{q}_s(t_1, \tau)$]

$$n\omega = \frac{1}{2}[\mathbf{q}_s(t_1, \tau) + \mathbf{A}(t_1)]^2 - \omega_{\mathbf{k}} + I_0. \quad (4)$$

We determine the maximum of this energy by the condition $\partial(n\omega)/\partial t_0 = 0$, i.e., by the condition that the electron is born at such time t_0 for which $n\omega$ has an extremum. This condition gives

$$\begin{aligned} E(t_0)[A(t_1) - A(t_0) + (t_1 - t_0)E(t_1)] \\ = p_0[E(t_1) - E(t_0)]. \end{aligned} \quad (5)$$

We find the extrema of $n\omega$ by solving the pair of equations (3) and (5) for t_0 and t_1 , $t_1 > t_0$ and introducing these solutions into Eq. (4). In Fig. 3(a) we present the results for the maximum value of n as a function of the ratio E_s/E_0 . The global maximum value of n for any value of E_s is slightly above 160 and, as E_s increases, n_{\max} for a particular value of E_s oscillates below this value with increasing amplitude. The optimal values of E_s are those for which n_{\max} equals the global maximum value. In Fig. 3(b) we present the return time which corresponds to n_{\max} , i.e., to the cutoff of the plateau in the DCS, as a function of the ratio E_s/E_0 . One sees that the return time increases exponentially with decreasing E_s . Because the T matrices contain the factor $\tau^{-3/2}$ [5], which corresponds to the spreading of the electron's wave packet, the probability of the electron's recombination is low for small E_s , and, therefore, the DCS is small for small E_s . This agrees with

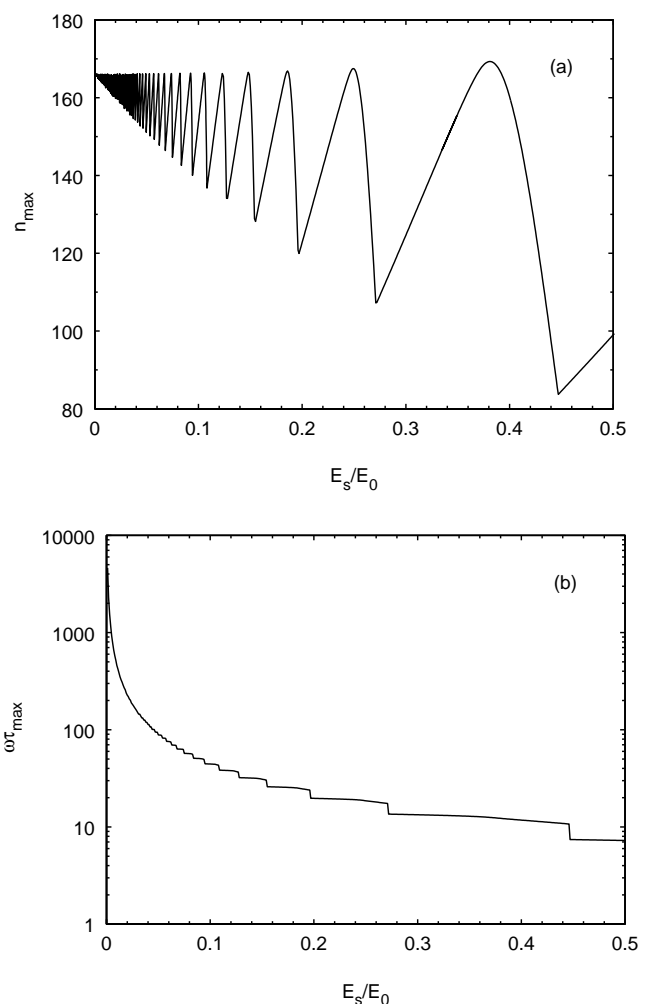


FIG. 3. Maximum value of the number n (a) and the corresponding return time τ (b), obtained using the quasiclassical method, as functions of the ratio of the static and the laser electric field strengths. The laser field parameters are the same as in Fig. 1.

our results in Fig. 2, i.e., that the plateau for positive values of n increases as E_s increases.

In order to explain why the plateau for positive values of n appears in the presence of a static field, we analyze Eq. (3) in more detail. Introducing new variables $\sigma = \omega\tau/2$ and $\varphi = \omega t_1$, the condition that the electron returns to the nucleus at time t_1 , Eq. (3), can be written as

$$a(\sigma)\sin(\varphi - \sigma) + b(\sigma)\cos(\varphi - \sigma) = c(\sigma), \quad (6)$$

where $a(\sigma) = \sin\sigma$, $b(\sigma) = \cos\sigma - \sin\sigma/\sigma$, and $c(\sigma) = (p_0/A_0) - \sigma E_s/E_0$. Equation (6) can be rewritten as a quadratic equation in the variable $x = \sin(\varphi - \sigma)$, and, therefore, for each τ we have two solutions for x . Introducing these solutions into Eq. (4), one obtains the number n as a function of the return time τ . For $E_s = 0$ there are no solutions of Eq. (6) because, in order that x is real, one must have $a^2 + b^2 \geq c^2$. But in our example $c^2 = (p_0/A_0)^2 = 1.734$, while the maximum of the function $a^2(\sigma) + b^2(\sigma)$ is only 1.5866.

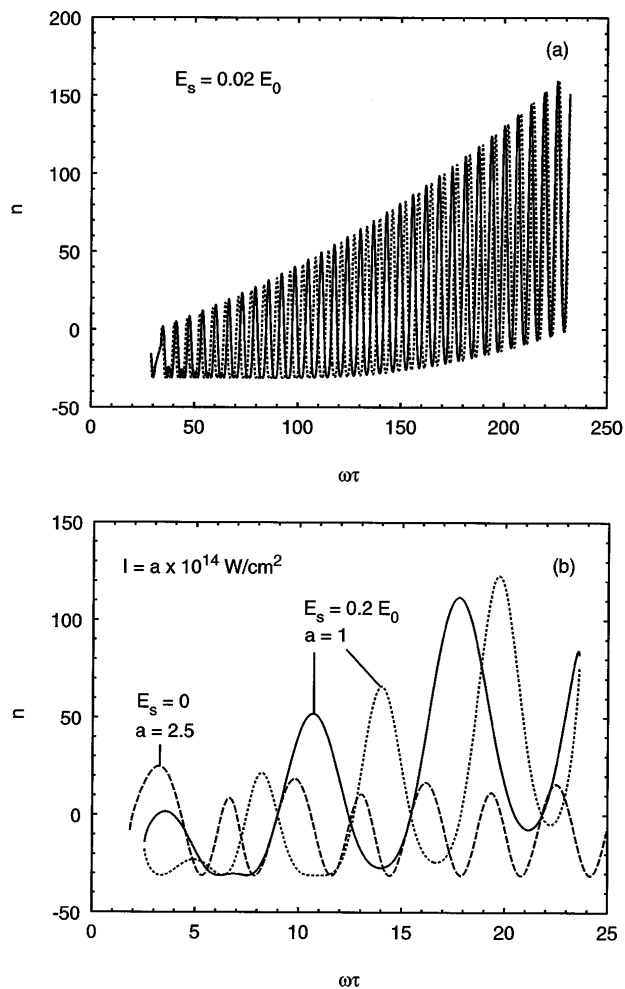


FIG. 4. The number n , Eq. (4), which corresponds to the solutions of Eq. (6), as a function of $\omega\tau$, for two different values of the static electric field strength: (a) $E_s = 0.02E_0$; (b) $E_s = 0.2E_0$. For each τ there are two solutions (represented by solid and dotted lines, respectively), which form pairs of maxima. The laser field parameters are the same as in Fig. 1, except for the dashed curve in (b), for which $E_s = 0$ and the laser field intensity is 2.5 times higher.

More precisely, if the electron initial kinetic energy $p_0^2/2 = \omega_K - I_0$ is larger than the maximum energy which the electron can acquire in the laser field (which is $3.17U_p$, the well-known cutoff law for high-order harmonic generation), then the laser field is not strong enough to return the electron to the nucleus. Therefore, the laser field alone (with $A_0 < 0.7939|p_0|$) is not capable of producing a positive n plateau in this case. But, in the presence of a static field parallel to \mathbf{p}_0 , the electron can be returned to the nucleus because the static field acts on it with the force $-E_s\hat{\mathbf{e}}$. In Fig. 4 we present the function $n = n(\omega\tau)$ for two different values of E_s : (a) $E_s = 0.02E_0$ and (b) $E_s = 0.2E_0$. The general structure of the function $n = n(\omega\tau)$ is that it has pairs of maxima, obtained by introducing the two solutions of Eq. (6) into Eq. (4) (represented in Fig. 4 by the solid and dotted lines). For small E_s the return time can be

long, while for larger E_s the return time is shorter. The kinetic energy which the electron acquires from the static field increases with the increase of the return time, and for $\tau > \tau_m$ the electron is no longer able to return to the nucleus [where in Fig. 4 $\omega\tau_m = 232$ (a) and 23.6 (b); for $\tau > \tau_m$ there are no solutions of Eq. (6)]. For $E_s = 0$, in the case when the laser field is strong enough that the condition $a^2 + b^2 \geq c^2$ is fulfilled, solutions of Eq. (6) exist. An example for $I = 2.5 \times 10^{14}$ W/cm² is presented in Fig. 4(b) by a dashed line. One sees that the number n , which determines the position of the plateau in the DCS, is smaller for $E_s = 0$ even though the laser field intensity is higher by a factor of 2.5. This is because the energy which the electron accumulates from the static field increases with τ .

We considered laser-assisted x-ray-atom scattering in the presence of a static electric field. The number of photons n exchanged with the laser field can be either even or odd. Our results show that the DCS as a function of n can have an extended plateau for positive values of n , indicating an increase of the energy of scattered x-ray photons by up to an order of magnitude. A quasiclassical explanation of these effects has also been presented.

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