

X-ray-atom scattering in the presence of a laser field

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We consider x-ray-hydrogen atom scattering in the presence of a monochromatic linearly polarized laser field. The S matrix of this process is presented and an expression for the differential cross section (DCS) is derived. We show that the time-dependent Wentzel-Kramers-Brillouin approximation can be applied to the present problem. The presented numerical results for the DCS as a function of the number n of photons exchanged with the laser field show a characteristic behavior. The number n can only be even. For $n=0, \pm 2$ we have pronounced maxima in the DCS, followed by sharp minima at $n=\pm 4$. After that, we have a plateau that is different for negative and positive values of n . The plateau for negative values of n is much more extended than for the positive ones. The structure of the plateau and the positions of the minima and maxima of the DCS do not depend on the laser field intensity, while the height of the plateaus strongly depends on it. We also analyze the dependence of the matrix elements of the x-ray spectra on the incident x-ray photon energies by using both the saddle-point method and the numerical evaluation, and we show that the shape and position of the plateau are determined by the simple relation $n\hbar\omega = I_0 - \hbar\omega_{\mathbf{K}}$. This condition connects the number of absorbed or emitted laser field photons n , the laser field photon energy $\hbar\omega$, the atomic ionization potential I_0 , and the energy of the incident x-ray photon $\hbar\omega_{\mathbf{K}}$. [S1050-2947(98)04909-9]

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I. INTRODUCTION

Investigations of atomic processes in the simultaneous presence of strong laser fields and soft-x-ray pulses are presently attracting considerable interest, both experimentally and theoretically. This is connected with the possibility of an efficient generation of high-order harmonics of the driving laser field. The latest reports [1,2] show that it is possible to generate harmonic photons of the energy 460 eV. The observation of the laser-assisted photoelectric effect [3] was just possible by using soft-x-ray pulses generated as high-order harmonics. There are also other schemes on which soft-x-ray lasers can operate (see [4,5] and references therein). There are only a small number of theoretical contributions to this field (see, for example, our recent work [6] on x-ray photoionization of hydrogen in the presence of a bichromatic laser field, and references therein). In the present contribution we shall consider x-ray scattering in the presence of a laser field. The number of publications concerning this process is even less than the number devoted to the laser-assisted x-ray photoionization process.

The elements of the x-ray scattering in the absence of a laser field can be found in the textbooks by Heitler [7] and by Loudon [8]. The differential cross section (DCS) for light scattering is expressed in the quantum-mechanical scattering theory by the Kramers-Heisenberg formula, which includes both elastic Rayleigh scattering and inelastic Raman scatter-

ing. If the photon energy $\hbar\omega_{\mathbf{K}}$ of the x ray is much larger than the atomic excitation energy (but still small enough so that the dipole approximation is valid [8]), then the DCS of elastic scattering corresponds to Thomson scattering and is given by the formula $(d\sigma/d\Omega)_{\text{Th}} = Z^2 r_e^2 (\hat{\mathbf{e}}_{\mathbf{K}} \cdot \hat{\mathbf{e}}_{\mathbf{K}'})^2$, where (in SI units) $r_e = e^2/(4\pi\epsilon_0 mc^2) = 2.8 \times 10^{-15}$ m is the classical electron radius, Z is the number of electrons in the atom, and $\hat{\mathbf{e}}_{\mathbf{K}}$ and $\hat{\mathbf{e}}_{\mathbf{K}'}$ are the unit polarization vectors of the incident and scattered photons, respectively. In the opposite case where $\hbar\omega_{\mathbf{K}}$ is much smaller than the atomic excitation energy (which we will not consider here), the elastic DCS is proportional to $\omega_{\mathbf{K}}^4$. The intermediate case is analyzed numerically for scattering by hydrogen in Gavrilá's work [9]. There are a lot of papers in which x-ray scattering by bound systems is considered in the absence of the laser field, of which we mention an early work by Levinger [10] and more recent work [11,12] on inelastic x-ray scattering (see also references in [12]). According to our knowledge, besides the references on x-ray photoionization mentioned in [6], x-ray scattering in the presence of a laser field was considered only in earlier work by Ehlötzky [13] and more recent work by Kálmán [14]. The latter is devoted to the laser-assisted inelastic x-ray scattering as a tool for determining the length of ultrafast x-ray pulses and is of no interest for our present work. For the laser-assisted x-ray scattering in the context of electron-atom collisions in a laser field, see the recent review article [15].

We shall first present the S -matrix theory of laser-assisted x-ray scattering in Sec. II. In Sec. III we introduce some approximations, explain their range of validity, and define the T matrices of the x-ray scattering processes. An expres-

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sion for the DCS for laser-assisted x-ray scattering is derived in Sec. IV. In Sec. V we apply the time-dependent WBK approximation to our problem and present our final expression for the DCS of laser-assisted x-ray scattering by hydrogen atoms. Section VI is devoted to the saddle-point method analysis of the x-ray spectra. Numerical results for a monochromatic linearly polarized laser field are presented in Sec. VII. Finally, Sec. VIII is devoted to the conclusions. All our results are derived in SI units. For a better estimate of the order of magnitude of the results obtained, we express the DCS in units of the Thomson DCS, which, for hydrogen atoms and parallel geometry, is equal to the square of the classical electron radius.

II. S-MATRIX THEORY

In order to derive an expression for the DCS of laser-assisted x-ray scattering, we start from a general form of the S -matrix,

$$S_{fi} = i\hbar \lim_{t' \rightarrow \infty} \lim_{t \rightarrow -\infty} \langle \Phi_{\text{out}}(t') | G(t', t) | \Phi_{\text{in}}(t) \rangle. \quad (1)$$

In Eq. (1), G is the total Green's operator, which corresponds to the total Hamiltonian

$$H = H_0 + e\mathbf{r} \cdot \mathbf{E}_x(t), \quad H_0 = \frac{\mathbf{p}^2}{2m} + V_A + e\mathbf{r} \cdot \mathbf{E}(t), \quad (2)$$

where $e\mathbf{r} \cdot \mathbf{E}_x(t)$ is the interaction of the atom with the x-ray field (in the length gauge and in the dipole approximation), $e\mathbf{r} \cdot \mathbf{E}(t)$ is the laser-atom interaction, also in the length gauge, and V_A is the atomic potential. We shall treat the laser field classically, so that, in the case of a linearly polarized monochromatic field, the laser electric field vector $\mathbf{E}(t)$ with the unit polarization vector $\hat{\mathbf{e}}$, frequency ω , and intensity I , is given by

$$\mathbf{E}(t) = E_0 \hat{\mathbf{e}} \sin \omega t, \quad I = \frac{1}{2} \varepsilon_0 c E_0^2. \quad (3)$$

In order to distinguish the x-ray field from the laser field, we shall consider the x-ray radiation field as quantized, i.e., according to [8], we define

$$\langle \Phi_f(t) | = i\hbar \langle \Phi_{\text{out}}(\infty) | \left(G_0(\infty, t) + \int dt' G_0(\infty, t') e\mathbf{r} \cdot \mathbf{E}_x(t') G(t', t) \right). \quad (8)$$

Substituting Eq. (8) into Eq. (7) and taking into account that $\langle 0_{\mathbf{K}} | \langle 1_{\mathbf{K}'} | \mathbf{E}_x(t) | 1_{\mathbf{K}} \rangle | 0_{\mathbf{K}'} \rangle = \mathbf{0}$ and that $\langle \Phi_{\text{out}}(\infty) | G_0(\infty, t) = (-i/\hbar) \langle \psi_f(t) | \langle 0_{\mathbf{K}} | \langle 1_{\mathbf{K}'} |$, we obtain

$$(S-1)_{fi} = -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt \int dt' \langle \psi_f(t') | \langle 0_{\mathbf{K}} | \langle 1_{\mathbf{K}'} | e\mathbf{r} \cdot \mathbf{E}_x(t') G(t', t) e\mathbf{r} \cdot \mathbf{E}_x(t) | \psi_i(t) | 1_{\mathbf{K}} \rangle | 0_{\mathbf{K}'} \rangle. \quad (9)$$

III. APPROXIMATIONS AND THE T -MATRICES

By now the only approximations we used were the nonrelativistic and the dipole approximation. They are satisfied for x-ray photon energies less than 100 eV, which we are considering [8]. Supposing that the x-ray field is not too strong, we obtain from Eq. (6) $G(t, t') \approx G_0(t, t')$. In this case, the remaining matrix elements in the vector space of the x-ray photons give the following result for the S matrix:

$$\mathbf{E}_x(t) = \mathbf{E}_x^{(+)}(t) + \mathbf{E}_x^{(-)}(t),$$

$$\mathbf{E}_x^{(+)}(t) = i \sum_{\mathbf{K}} \left(\frac{\hbar \omega_{\mathbf{K}}}{2\varepsilon_0 V} \right)^{1/2} \hat{\mathbf{e}}_{\mathbf{K}} a_{\mathbf{K}} e^{-i\omega_{\mathbf{K}} t}, \quad (4)$$

$$\mathbf{E}_x^{(-)}(t) = -i \sum_{\mathbf{K}} \left(\frac{\hbar \omega_{\mathbf{K}}}{2\varepsilon_0 V} \right)^{1/2} \hat{\mathbf{e}}_{\mathbf{K}} a_{\mathbf{K}}^{\dagger} e^{i\omega_{\mathbf{K}} t},$$

where $a_{\mathbf{K}}$ and $a_{\mathbf{K}}^{\dagger}$ are the annihilation and creation operators of the x-ray field photons corresponding to the wave vectors \mathbf{K} , frequencies $\omega_{\mathbf{K}}$, and unit polarization vectors $\hat{\mathbf{e}}_{\mathbf{K}}$. $V = L^3$ is the quantization volume. We consider the scattering of an x-ray photon with the initial wave vector \mathbf{K} and energy $\hbar \omega_{\mathbf{K}}$ into a final state with the wave vector \mathbf{K}' and energy $\hbar \omega_{\mathbf{K}'}$. If we denote the initial and the final atomic state vectors and ionization energies by $|\psi_0\rangle$ and I_0 , respectively, then the *in* and *out* states, which appear in Eq. (1), can be written as

$$|\Phi_{\text{in}}(t)\rangle = |\psi_0\rangle e^{iI_0 t/\hbar} |1_{\mathbf{K}}\rangle |0_{\mathbf{K}'}\rangle, \quad (5)$$

$$|\Phi_{\text{out}}(t)\rangle = |\psi_0\rangle e^{iI_0 t/\hbar} |0_{\mathbf{K}}\rangle |1_{\mathbf{K}'}\rangle.$$

The total Green's operator satisfies the Lippmann-Schwinger equation

$$G(t, t') = G_0(t, t') + \int dt'' G(t, t'') e\mathbf{r} \cdot \mathbf{E}_x(t'') G_0(t'', t'), \quad (6)$$

where the Green's operator G_0 of the Hamiltonian H_0 operates in the vector space of x-ray photons as a unit operator. Introducing Eq. (6) into Eq. (1) and taking into account that the total Green's operator, by acting on the *out* state, yields a total final state at the time t of the form $\langle \Phi_f(t) | = i\hbar \langle \Phi_{\text{out}}(\infty) | G(\infty, t)$, while the operator G_0 only acts on the atomic part of the *in* state as $i\hbar G_0(t, -\infty) |\psi_0\rangle \exp(iI_0 t/\hbar) = |\psi_i(t)\rangle$, we obtain

$$(S-1)_{fi} = -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt \langle \Phi_f(t) | e\mathbf{r} \cdot \mathbf{E}_x(t) | \psi_i(t) | 1_{\mathbf{K}} \rangle | 0_{\mathbf{K}'} \rangle. \quad (7)$$

By applying Eq. (6), once more we get for the final state

$$(S-1)_{fi} = -\frac{i}{\hbar} \frac{\hbar e^2}{2\varepsilon_0 V} (\omega_{\mathbf{K}} \omega_{\mathbf{K}'})^{1/2} \int_{-\infty}^{\infty} dt \int dt' \{ \langle \psi_f(t') | \mathbf{r} \cdot \hat{\mathbf{e}}_{\mathbf{K}} G_0(t', t) \mathbf{r} \cdot \hat{\mathbf{e}}_{\mathbf{K}'} | \psi_i(t) \rangle e^{-i\omega_{\mathbf{K}'} t' + i\omega_{\mathbf{K}} t} \\ + \langle \psi_f(t') | \mathbf{r} \cdot \hat{\mathbf{e}}_{\mathbf{K}'} G_0(t', t) \mathbf{r} \cdot \hat{\mathbf{e}}_{\mathbf{K}} | \psi_i(t) \rangle e^{i\omega_{\mathbf{K}'} t' - i\omega_{\mathbf{K}} t} \}. \quad (10)$$

Our next approximation is to neglect the laser field dressing of the initial and final states, i.e., the substitution $|\psi_j(t)\rangle \approx |\psi_0\rangle \exp(iI_0 t/\hbar)$, $j=i,f$. This approximation is valid for the laser field intensities much less than the atomic unit of intensity $I_A = 3.51 \times 10^{16}$ W/cm², which is satisfied in our case. Furthermore, we have shown in our previous paper [6] that the first-order corrections, obtained for these wave functions from the time-dependent perturbation theory, give only small contributions to the DCS of photoionization processes. Using these approximations and transforming the integrals over the times in Eq. (10) by means of the identity $\int_{-\infty}^{\infty} dt \int_t^{\infty} dt' f(t', t) = \int_{-\infty}^{\infty} dt' \int_{-\infty}^{t'} dt f(t', t)$, upon introducing the new variables $t'' = t'$, $\tau = t' - t$, and writing t instead of t'' in the final expression, we obtain

$$(S-1)_{fi} = -\frac{i}{\hbar} \frac{\hbar e^2}{2\varepsilon_0 V} (\omega_{\mathbf{K}} \omega_{\mathbf{K}'})^{1/2} \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau e^{-iI_0 t/\hbar} \langle \psi_0 | \{ \mathbf{r} \cdot \hat{\mathbf{e}}_{\mathbf{K}} e^{-i\omega_{\mathbf{K}} t} G_0(t, t-\tau) \mathbf{r} \cdot \hat{\mathbf{e}}_{\mathbf{K}'} e^{i\omega_{\mathbf{K}'}(t-\tau)} \\ + \mathbf{r} \cdot \hat{\mathbf{e}}_{\mathbf{K}'} e^{i\omega_{\mathbf{K}'} t} G_0(t, t-\tau) \mathbf{r} \cdot \hat{\mathbf{e}}_{\mathbf{K}} e^{-i\omega_{\mathbf{K}}(t-\tau)} \} | \psi_0 \rangle e^{iI_0(t-\tau)/\hbar}. \quad (11)$$

Our next approximation is to neglect in Eq. (11) the influence of the Coulomb field on the intermediate propagator, i.e., to replace the Green's operator G_0 by the Volkov Green's operator

$$G_0(t, t-\tau) \approx -\frac{i}{\hbar} \int d\mathbf{q} |\chi_{\mathbf{q}}(t)\rangle \langle \chi_{\mathbf{q}}(t-\tau)|, \quad (12)$$

where the Volkov state vectors in the length gauge are $[\mathbf{E}(t) = -\partial \mathbf{A}(t)/\partial t, e = |e\rangle]$

$$|\chi_{\mathbf{q}}(t)\rangle = |\mathbf{q} + \frac{e}{\hbar} \mathbf{A}(t)\rangle \exp(-i\{\mathbf{q} \cdot \boldsymbol{\alpha}(t) + [\mathcal{U}(t) + E_{\mathbf{q}} t]/\hbar\}), \quad (13)$$

with

$$\boldsymbol{\alpha}(t) = \frac{e}{m} \int_{t-\tau}^t dt' \mathbf{A}(t'), \quad \mathcal{U}(t) = \frac{e^2}{2m} \int_{t-\tau}^t dt' \mathbf{A}^2(t') = \mathcal{U}_1(t) + U_p t, \quad (14)$$

where $U_p = e^2 A_0^2 / 4m$ is the ponderomotive potential, $E_{\mathbf{q}} = \hbar^2 \mathbf{q}^2 / 2m$, and $A_0 = E_0 / \omega$. This approximation was successfully used in the analysis of high-order harmonics generation [16,17] and above-threshold ionization [18,19]. The corrections to this approximation can be obtained by replacing the Volkov waves by the Coulomb-Volkov waves or by the laser-field modified Coulomb-Volkov waves, but we shall not consider this here (see [6] and references therein). The quasiclassical action that corresponds to the propagation from the atomic ground state at time $t-\tau$ to the ground state at time t is

$$S(\mathbf{q}; t, \tau) = \int_{t-\tau}^t dt' \left\{ \frac{\hbar^2}{2m} \left(\mathbf{q} + \frac{e}{\hbar} \mathbf{A}(t') \right)^2 + I_0 \right\} = (E_{\mathbf{q}} + I_0 + U_p) \tau + \hbar \mathbf{q} \cdot [\boldsymbol{\alpha}(t) - \boldsymbol{\alpha}(t-\tau)] + \mathcal{U}_1(t) - \mathcal{U}_1(t-\tau). \quad (15)$$

Both matrix elements that appear in Eq. (11) contain the factor $\exp[-i(\omega_{\mathbf{K}} - \omega_{\mathbf{K}'})t]$. Taking into account that $\mathbf{E}(t)$, $\mathbf{A}(t)$, $\boldsymbol{\alpha}(t)$, $\mathcal{U}_1(t)$, and $S(\mathbf{q}; t, \tau)$ are $2\pi/\omega$ -periodic functions of t , the remaining part of the two matrix elements mentioned above can be written in the form $C_{\mathbf{K}, \mathbf{K}'} \mathcal{T}_{\mathbf{K}, \mathbf{K}'}^{(\pm)}(\varphi)$, with $C_{\mathbf{K}, \mathbf{K}'} = (\hbar e^2 / 2\varepsilon_0 V) (\omega_{\mathbf{K}} \omega_{\mathbf{K}'})^{1/2}$, and $\varphi = \omega t$, while

$$\mathcal{T}_{\mathbf{K}, \mathbf{K}'}^{(\pm)}(\varphi) = \int_0^{\infty} d\tau \int d\mathbf{q} \left\langle \psi_0 | \mathbf{r} \cdot \hat{\mathbf{e}}_{\mathbf{K}} \left| \mathbf{q} + \frac{e}{\hbar} \mathbf{A}(t) \right\rangle \left\langle \mathbf{q} + \frac{e}{\hbar} \mathbf{A}(t-\tau) | \mathbf{r} \cdot \hat{\mathbf{e}}_{\mathbf{K}'} | \psi_0 \right\rangle \exp\{-i[S(\mathbf{q}; t, \tau)/\hbar \pm \omega_{\mathbf{K}'} \tau]\}, \quad (16)$$

so that

$$(S-1)_{fi} = (-i/\hbar)^2 C_{\mathbf{K}, \mathbf{K}'} \int_{-\infty}^{\infty} dt [\mathcal{T}_{\mathbf{K}, \mathbf{K}'}^{(+)}(\varphi) + \mathcal{T}_{\mathbf{K}', \mathbf{K}}^{(-)}(\varphi)] \exp[-i(\omega_{\mathbf{K}} - \omega_{\mathbf{K}'})t]. \quad (17)$$

By expanding the matrix elements $\mathcal{T}_{\mathbf{K},\mathbf{K}'}^{(\pm)}(\varphi)$ into the Fourier series

$$\mathcal{T}_{\mathbf{K},\mathbf{K}'}^{(\pm)}(\varphi) = \sum_{n=-\infty}^{\infty} T_{\mathbf{K},\mathbf{K}'}^{(\pm)}(n) \exp(-in\varphi), \quad (18)$$

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

we obtain

$$(S-1)_{fi} = (-i/\hbar)^2 C_{\mathbf{K},\mathbf{K}'} 2\pi \sum_n \delta(\omega_{\mathbf{K}'} - \omega_{\mathbf{K}} - n\omega) T_{fi}(n), \quad (19)$$

$$T_{fi}(n) = T_{\mathbf{K},\mathbf{K}'}^{(+)}(n) + T_{\mathbf{K}',\mathbf{K}}^{(-)}(n).$$

The physical meaning of the two T -matrix elements in Eq. (19) is the following. The matrix element $T_{\mathbf{K}',\mathbf{K}}^{(-)}(n)$ corresponds to the processes in which an x-ray photon of the wave vector \mathbf{K} and energy $\hbar\omega_{\mathbf{K}}$ is absorbed first. The atom gets ionized and the electron propagates under the influence of the laser field only during the time interval from $t-\tau$ to t when it comes back to the atomic core (i.e., the return time τ). At this instant the electron recombines, exchanging n photons with the laser field and emitting an x-ray photon of the wave vector \mathbf{K}' and of the energy $\hbar\omega_{\mathbf{K}'} = \hbar\omega_{\mathbf{K}} + n\hbar\omega$. For the matrix element $T_{\mathbf{K},\mathbf{K}'}^{(+)}(n)$ we have first the emission

of the x-ray photon of the wave vector \mathbf{K}' and the energy $\hbar\omega_{\mathbf{K}'}$, then the electron propagation, and, finally, the absorption (or emission) of n photons of the laser field and the absorption of one x-ray photon of the wave vector \mathbf{K} and the energy $\hbar\omega_{\mathbf{K}}$.

IV. DIFFERENTIAL CROSS-SECTION

The rate (probability per unit time) of emission of x-ray photons of frequencies within the interval $(\omega_{\mathbf{K}'} - \varepsilon, \omega_{\mathbf{K}'} + \varepsilon)$ and with the polarization $\hat{\mathbf{e}}_{\mathbf{K}'}$ into a solid angle $d\Omega_{\hat{\mathbf{K}'}}$ is [8]

$$w_{fi} d\Omega_{\hat{\mathbf{K}'}} = \frac{1}{T_p} \frac{V}{(2\pi c)^3} d\Omega_{\hat{\mathbf{K}'}} \int_{\omega_{\mathbf{K}'} - \varepsilon}^{\omega_{\mathbf{K}'} + \varepsilon} d\omega_{\mathbf{K}} \omega_{\mathbf{K}}^2 |(S-1)_{fi}|^2, \quad (20)$$

where the connection $\Sigma_{\vec{k}} \rightarrow [V/(2\pi)^3] \int d\mathbf{K} = [V/(2\pi c)^3] \int d\omega_{\mathbf{K}} \omega_{\mathbf{K}}^2 \int d\Omega_{\hat{\mathbf{K}}}$ was used, and ε is small enough so that $\omega_{\mathbf{K}}^2 |(S-1)_{fi}|^2$ is almost constant in the interval of integration. T_p is the laser field pulse duration time. The time duration of x-ray pulses generated in high-order harmonic generation processes is usually shorter than the duration of the laser field pulse. Hence one can assume that the x-ray scattering process happens at some instant $t_s \in [0, T_p]$. According to Eq. (19), we obtain for the absolute square of the S -matrix element

$$\begin{aligned} |(S-1)_{fi}|^2 &= \left(\frac{2\pi}{\hbar^2} C_{\mathbf{K},\mathbf{K}'} \right)^2 \sum_n T_{fi}(n) \delta(\omega_{\mathbf{K}'} - \omega_{\mathbf{K}} - n\omega) \sum_{n'} T_{fi}^*(n') \delta(\omega_{\mathbf{K}'} - \omega_{\mathbf{K}} - n'\omega) \\ &= \frac{T_p}{2\pi} \left(\frac{2\pi}{\hbar^2} C_{\mathbf{K},\mathbf{K}'} \right)^2 \sum_n |T_{fi}(n)|^2 \delta(\omega_{\mathbf{K}'} - \omega_{\mathbf{K}} - n\omega), \end{aligned} \quad (21)$$

where we used the relation $2\pi\delta(0) = T_p$ (for $T_p \rightarrow \infty$). The differential cross section can be obtained by dividing the emission rate $w_{fi}(n)$ by the incident x-ray photon flux $j_{\mathbf{K}} = c/V$. Taking into account the quantity $C_{\mathbf{K},\mathbf{K}'}$, defined above Eq. (16), we obtain

$$\frac{d\sigma(n)}{d\Omega_{\hat{\mathbf{K}'}}} = \left(\frac{e^2}{4\pi\varepsilon_0\hbar} \right)^2 K K'^3 |T_{fi}(n)|^2, \quad \omega_{\mathbf{K}'} = \omega_{\mathbf{K}} + n\omega, \quad (22)$$

where $K = \omega_{\mathbf{K}}/c$, $K' = \omega_{\mathbf{K}'}/c$, and the energy conserving condition $\hbar\omega_{\mathbf{K}'} = \hbar\omega_{\mathbf{K}} + n\hbar\omega$ comes from the argument of the δ function. This is our final result for the DCS of x-ray scattering with the absorption ($n > 0$) or emission ($n < 0$) of n laser photons.

V. TIME-DEPENDENT WBK APPROXIMATION

In order to determine the DCS we have to compute the T matrices that are the Fourier components of the matrix ele-

ments $\mathcal{T}_{\mathbf{K},\mathbf{K}'}^{(\pm)}(\varphi)$ defined by Eq. (16). The three-dimensional integral over the intermediate electron momenta $\hbar\mathbf{q}$ can be computed using the saddle-point method, similarly as in [17]. Denoting the subintegral matrix elements by $h(\mathbf{q}; t, \tau)$, we obtain ($\mathbf{p} = \hbar\mathbf{q}$) the result

$$\begin{aligned} &\hbar^3 \int d\mathbf{q} h(\mathbf{q}; t, \tau) \exp[-iS(\mathbf{q}; t, \tau)/\hbar] \\ &= \left(\frac{2\pi m\hbar}{i\tau} \right)^{3/2} \exp[-iS(\mathbf{q}_s; t, \tau)/\hbar] \\ &\quad \times \left(1 - i \frac{m\hbar}{2\tau} \frac{\partial^2}{\hbar^2 \partial \mathbf{q}^2} + \dots \right) h(\mathbf{q}; t, \tau) \Big|_{\mathbf{q}=\mathbf{q}_s(t, \tau)}, \end{aligned} \quad (23)$$

where the stationary momentum $\hbar\mathbf{q}_s$,

$$\hbar \mathbf{q}_s(t, \tau) = -\frac{e}{\tau} \int_{t-\tau}^t dt' \mathbf{A}(t') = \frac{m}{\tau} [\boldsymbol{\alpha}(t-\tau) - \boldsymbol{\alpha}(t)], \quad (24)$$

is the solution of the equation $\nabla_{\mathbf{q}} S(\mathbf{q}; t, \tau) = \mathbf{0}$. The result (23) is a version of the time-dependent WBK approximation [20]. We have shown previously in the context of the high-order harmonic generation and above-threshold ionization within the strong-field approximation [17–19] that satisfactory results can be obtained by keeping only the zeroth-order term of the expansion of the form (23). For the processes mentioned, the number of the exchanged photons is large. It will be worthwhile to check whether this approximation is applicable for relatively small n , which we shall consider here. In order to verify this, we computed the first-order correction (the term with $\partial^2/\partial \mathbf{q}^2$) and found that this approximation is satisfactory for $|n| > 2$. This is an unexpected result that shows that the above approximation, Eq. (23), has a wider range of applicability than it was believed previously. The matrix elements that appear in $T_{\mathbf{K}, \mathbf{K}'}^{(\pm)}(\varphi)$ are of the form (for a hydrogen atom in its ground state $|\psi_0\rangle$)

$$\langle \mathbf{q} | \hat{\mathbf{e}}_{\mathbf{K}} \cdot \mathbf{r} | \psi_0 \rangle = -i \frac{2^{7/2} \mathbf{q} \cdot \hat{\mathbf{e}}_{\mathbf{K}}}{\pi a_B^{5/2} (\mathbf{q}^2 + a_B^{-2})^3}, \quad (25)$$

where a_B is the Bohr radius. In the case of a linearly polarized laser field we have $\mathbf{q} = q_s \hat{\mathbf{e}}$, so that the DCS contains the factor $(\hat{\mathbf{e}} \cdot \hat{\mathbf{e}}_{\mathbf{K}})^2 (\hat{\mathbf{e}} \cdot \hat{\mathbf{e}}_{\mathbf{K}'})^2$. This factor has its maximum (equal to 1) for parallel geometry: $\hat{\mathbf{e}} \parallel \hat{\mathbf{e}}_{\mathbf{K}} \parallel \hat{\mathbf{e}}_{\mathbf{K}'}$. Therefore, in order to simplify the situation, we shall compute our numerical results for this geometry only.

Our final result for the DCS, for which we shall present the numerical result, is given by Eq. (22), in which

$$T_{fi}(n) = T_{\mathbf{K}, \mathbf{K}'}^{(+)}(n) + T_{\mathbf{K}', \mathbf{K}}^{(-)}(n), \quad (26)$$

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

where the $\mathcal{T}_{\mathbf{K}, \mathbf{K}'}^{(\pm)}(\varphi)$ are given by Eq. (16). According to Eq. (25), for the parallel geometry the zeroth-order term of the WBK expansion (23) yields

$$\begin{aligned} \mathcal{T}_{\mathbf{K}, \mathbf{K}'}^{(\pm)(0)}(\varphi) = & - \left(\frac{2\pi m}{i\hbar} \right)^{3/2} \frac{2^7}{\pi^2 a_B^5} \int_0^\infty \frac{d\tau}{\tau^{3/2}} \exp\{-i[S(\mathbf{q}_s; t, \tau) \pm \hbar \omega_{\mathbf{K}', \mathbf{K}}] / \hbar\} \\ & \times \frac{\left(q_s + \frac{e}{\hbar} A(t) \right) \left(q_s + \frac{e}{\hbar} A(t-\tau) \right)}{\left[\left(q_s + \frac{e}{\hbar} A(t) \right)^2 + a_B^{-2} \right]^{3/2} \left[\left(q_s + \frac{e}{\hbar} A(t-\tau) \right)^2 + a_B^{-2} \right]^{3/2}}, \end{aligned} \quad (27)$$

where S and $\mathbf{q}_s \equiv q_s \hat{\mathbf{e}}$ are given by Eqs. (15) and (24), respectively, and $\mathbf{A}(t) \equiv A(t) \hat{\mathbf{e}}$.

VI. SADDLE-POINT METHOD ANALYSIS OF THE X-RAY SPECTRA

According to Eqs. (19) and (22), the DCS for scattering in a laser field is determined by the T matrix $T_{fi}(n) = T_{\mathbf{K}, \mathbf{K}'}^{(+)}(n) + T_{\mathbf{K}', \mathbf{K}}^{(-)}(n)$. The matrix elements $T_{\mathbf{K}, \mathbf{K}'}^{(\pm)}(n)$ can be evaluated by computing the five-dimensional integral over the time t , the return time τ , and the intermediate electron momenta \mathbf{q} . We have shown in the preceding section that the three-dimensional integral over the intermediate electron momenta can be replaced by an infinite sum of the matrix elements. The remaining integrals can also be analyzed by applying the saddle-point method. The behavior of all these matrix elements is mainly determined by the factors that appear in the exponent. According to Eqs. (16)–(18) and (23), we have

$$\begin{aligned} T_{\mathbf{K}, \mathbf{K}'}^{(\pm)}(n) \propto & \int dt \int d\tau \tau^{-3/2} h(\mathbf{q}_s; t, \tau) \\ & \times \exp\{-i[S(\mathbf{q}_s; t, \tau) / \hbar \pm \omega_{\mathbf{K}', \mathbf{K}} \tau - n\omega t]\}. \end{aligned} \quad (28)$$

By applying the saddle-point method to the integral over the time t , we obtain the condition $\partial S / \partial t = n\hbar\omega$, which can be written in the form

$$\frac{\boldsymbol{\pi}^2(t)}{2m} - \frac{\boldsymbol{\pi}^2(t-\tau)}{2m} = n\hbar\omega, \quad (29)$$

where $\boldsymbol{\pi}(t') = \hbar \mathbf{q}_s(t, \tau) + e\mathbf{A}(t')$ is the momentum of the electron in the laser field at time t' . The second condition can be obtained by applying the saddle-point method to the integral over τ . This condition depends on the T -matrix element that we are considering, and it is, respectively,

$$\begin{aligned} \frac{\boldsymbol{\pi}^2(t-\tau)}{2m} &= -\hbar\omega_{\mathbf{K}'} - I_0 \quad \text{for } T_{\mathbf{K}, \mathbf{K}'}^{(+)}(n), \\ \frac{\boldsymbol{\pi}^2(t-\tau)}{2m} &= +\hbar\omega_{\mathbf{K}} - I_0 \quad \text{for } T_{\mathbf{K}', \mathbf{K}}^{(-)}(n). \end{aligned} \quad (30)$$

The right-hand side of the first of the above equations is always negative, so that the solutions for t and τ are complex. A similar condition was obtained in the context of the analysis of the cutoff law in high-order harmonic generation [16,17]. The more interesting is the second condition of Eq. (30), because for $\hbar\omega_{\mathbf{K}} \geq I_0$ it corresponds to real times t and

τ . By using numerical examples we shall show in the next section that this term essentially determines the behavior of the final x-ray spectra. The matrix element $T_{\mathbf{K}',\mathbf{K}}^{(-)}(n)$ corresponds to a process in which an x-ray photon is absorbed first. For $\hbar\omega_{\mathbf{K}} \geq I_0$ the electron can really be ionized and it has the energy $\pi^2(t-\tau)/2m$ in the laser field at the instant $t-\tau$. Then this electron moves under the influence of the laser field only. At some time t it gets close to the atomic core and can be recaptured by the nucleus. The recombination process is the most probable one for low electron energies, i.e., for $\pi^2(t-\tau)/2m \approx 0$. Introducing this condition into Eq. (29), we obtain $\pi^2(t-\tau)/2m = -n\hbar\omega$, which, in combination with the second condition in Eq. (30), gives

$$n\hbar\omega = I_0 - \hbar\omega_{\mathbf{K}}. \quad (31)$$

We, therefore, obtained a simple linear dependence that connects the number of absorbed (or emitted) laser field photons n , the atomic ionization potential I_0 , and the energy of the incident x-ray photon $\hbar\omega_{\mathbf{K}}$. Besides this condition, one should take into account the energy conserving condition $\hbar\omega_{\mathbf{K}'} = \hbar\omega_{\mathbf{K}} + n\hbar\omega \geq 0$, which determines the cutoff of the spectrum at large negative values of n , and, according to symmetry and parity considerations of the matrix elements, that moreover the number of the exchanged photons n must be even. We shall show in the next section that the x-ray spectrum is mainly determined by these conditions. The condition (31), and, therefore, the values of n that characterize the spectrum, do not depend on the intensity of the laser field. As we shall show, the DCS increases with the increase of the laser field intensity, but the general shape of the spectrum is determined by the simple condition (31).

VII. NUMERICAL RESULTS

We shall first check whether our time-dependent WBK approximation gives reasonable results. In Fig. 1 we present our data for the laser-assisted x-ray scattering DCS in units of r_e^2 as functions of the number of photons exchanged with the laser field, for two values of the laser field intensity. The triangles and squares represent the results obtained using the zeroth- and the first-order term of the WBK expansion (23), while the dotted and the dashed line correspond to the zeroth-order term only. As one can see, for $|n| > 2$, the zeroth-order approximation gives satisfactory results. Beside this, the results presented in Fig. 1 show a typical behavior of the x-ray spectra that we obtained in the present paper. First, only an even number of laser field photons is absorbed or emitted. Next, for $n=0, \pm 2$ we have a pronounced maximum in the spectrum and then a rapid drop at $n = \pm 4$. After that, there is a plateau that is quite different for the positive and the negative values of n . The height of the plateau is determined by the laser field intensity. The plateau for positive n is small (almost negligible) in comparison with the plateau for the negative values of n . In Fig. 2 we analyze the contributions of the matrix elements $T_{\mathbf{K},\mathbf{K}'}^{(+)}(n)$ and $T_{\mathbf{K}',\mathbf{K}}^{(-)}(n)$ to the DCS. The results denoted by “a” correspond to the matrix elements $T_{\mathbf{K},\mathbf{K}'}^{(-)}(n)$ and to the processes in which an x-ray photon is absorbed first, while the results denoted by “e” correspond to the $T_{\mathbf{K},\mathbf{K}'}^{(+)}(n)$ and to the pro-

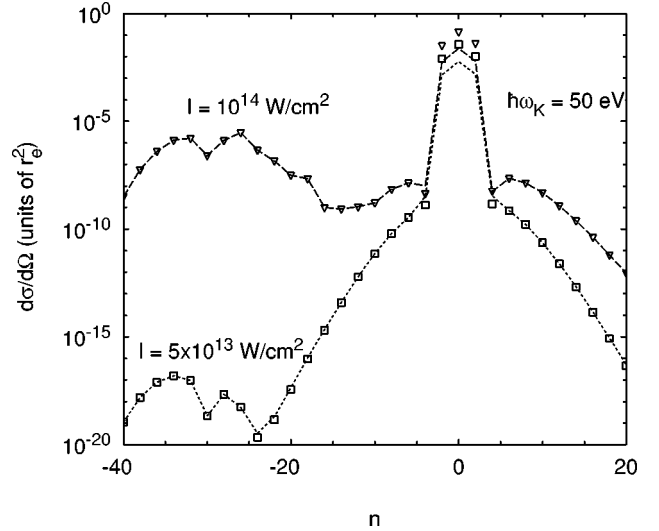


FIG. 1. The DCS of x-ray scattering in units of r_e^2 ($r_e = 2.8 \times 10^{-15}$ m is the classical electron radius) as functions of the number n of absorbed (or emitted) laser field photons, for two values of the laser field intensity: $I = 5 \times 10^{13}$ W/cm² (squares and dotted curve) and $I = 10^{14}$ W/cm² (triangles and dashed curve). The laser field is linearly polarized and monochromatic with the photon energy $\hbar\omega = 1.17$ eV. The energy of the incident x-ray photons is $\hbar\omega_{\mathbf{K}} = 50$ eV. The results presented by the dotted and dashed curves are obtained using the zeroth-order term of the WBK approximation (see text), while the triangles and squares correspond to the results that are obtained taking into account the first-order correction.

cesses in which we have first the emission of an x-ray photon. We see that the “e” spectrum is symmetric with respect to $n=0$, while the “a” spectrum has a broad plateau for the negative values of n . Therefore, the x-ray spectra are mainly determined by the process in which we have the absorption

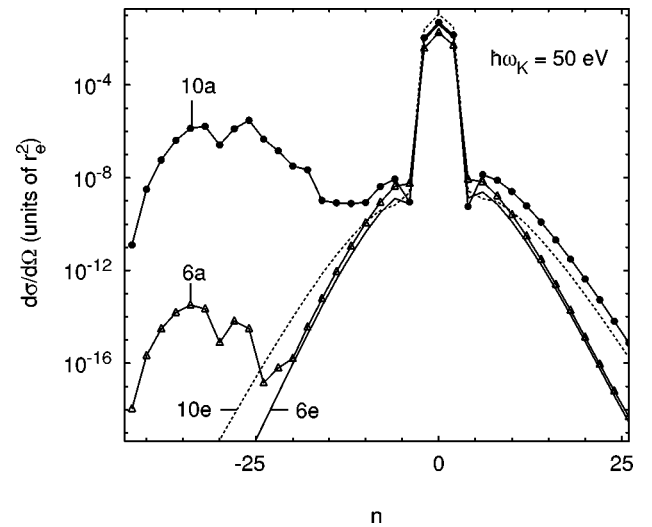


FIG. 2. The DCS of x-ray scattering in the presence of a laser field presented as in Fig. 1. The curves denoted by 6 and 10 correspond to the laser field intensities $I = 6 \times 10^{13}$ W/cm² and $I = 10^{14}$ W/cm², respectively. The results obtained using only the matrix element that corresponds to the processes in which an x-ray photon is absorbed first are denoted by the letter “a,” while the letter “e” corresponds to the processes in which we have first the emission of an x-ray photon.

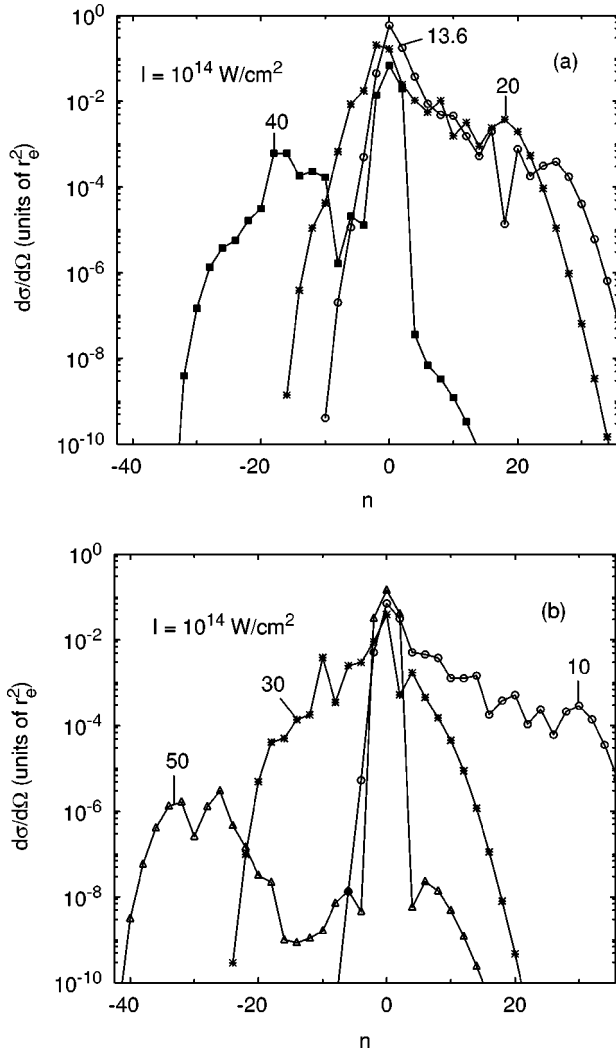


FIG. 3. The DCS of x-ray scattering presented as in Figs. 1 and 2. The presented results are obtained by including both the zeroth- and the first-order term of the WKB approximation, and by using both T -matrix elements. The laser field intensity is $I = 10^{14}$ W/cm². (a) The results for the following values of the incident x-ray photon energies: 13.6 eV, 20 eV, and 40 eV are presented, while for (b) the incident x-ray photon energies are 10 eV, 30 eV, and 50 eV.

of the x-ray photon first, which is in accordance with our analysis presented in the preceding section. For the results shown in Figs. 1 and 2 the incident x-ray photon energy was fixed to $\hbar\omega_{\mathbf{K}} = 50$ eV and the laser field photon energy to $\hbar\omega = 1.17$ eV, while the laser field intensities were $I = 5 \times 10^{13}$ W/cm², $I = 6 \times 10^{13}$ W/cm², and $I = 10^{14}$ W/cm². In Fig. 3 we present the DCS for a fixed laser field intensity, but for different values of $\hbar\omega_{\mathbf{K}}$. The spectra for $\hbar\omega_{\mathbf{K}} = 30$ eV, 40 eV, and 50 eV are similar to the one presented in Figs. 1 and 2, while for $\hbar\omega_{\mathbf{K}} = 10$ eV, 13.6 eV, and 20 eV the spectra are different. In the latter case, the cutoff for the negative values of n appears earlier (i.e., for smaller values of $|n|$) due to the energy conserving condition, and the plateau is shifted to the positive values of n . A sharp maximum appears for $\hbar\omega_{\mathbf{K}} = I_0$ and $n = 0$. Finally, in Fig. 4 we present as a function of the incident x-ray photon energy $\hbar\omega_{\mathbf{K}}$ those numbers of photons n , exchanged with the laser field, for which the DCS of x-ray scattering have their first minimum before the

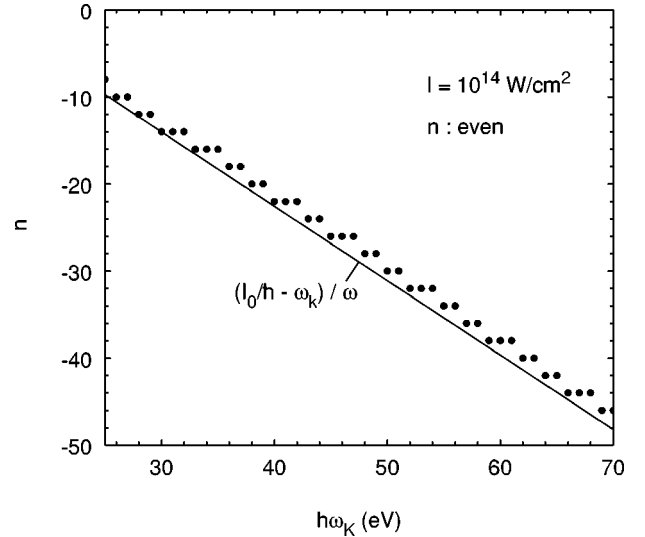


FIG. 4. The dots represent as a function of the incident x-ray photon energies $\hbar\omega_{\mathbf{K}}$ those numbers of photons n , exchanged with the laser field, for which the DCS of x-ray scattering have their first minima before the cutoff of the spectrum for large negative values of n . The laser field intensity is $I = 10^{14}$ W/cm². On this figure is also presented a straight line denoted by $(I_0/\hbar - \omega_{\mathbf{K}})/\omega$. The equation $n\hbar\omega = I_0 - \hbar\omega_{\mathbf{K}}$ follows from the saddle-point method analysis of the T -matrix elements (see text).

cutoff of the spectrum for large negative values of n . For the general shape of the plateau for negative values of n , see, for example, the curve 10a in Fig. 2. We have chosen to present the positions of these minima because they can be easily extracted from the spectra. We have also presented for comparison a straight line denoted by $(I_0/\hbar - \omega_{\mathbf{K}})/\omega$, which is determined by the condition (31), which we obtained in the preceding section. Our numerical results follow precisely this line. The agreement is even better if one takes into account that the number n can only be an even integer.

VIII. CONCLUSIONS

Only a little work has been devoted so far to x-ray-atom scattering in the presence of a laser field. We presented in our present work the S -matrix theory of this process, which, after suitable approximations, leads to a relatively simple expression for the DCS, Eq. (22). The T -matrix element contained in this expression consists of two terms that can be explained using two Feynman diagrams: one corresponds to the processes in which the x-ray photon is absorbed first, while for the other the x-ray photon is emitted first. The intermediate propagator between the absorption and the emission of the x-ray photon is dressed by the laser field so that, by taking into account the parity conservation condition, in x-ray-atom scattering in a laser field an even number of the laser field photons can be absorbed or emitted only. This is obvious because the atom experiences no change of state due to the combined effects of x-ray and laser scattering. We have shown that the expression obtained for the DCS can be further simplified by applying a particular version of the time-dependent WKB approximation. This method was developed within the strong-field approximation in the context of high-order harmonics generation [16,17]

and above-threshold ionization [18,19] and it is assumed to be applicable in cases where the number of exchanged photons n is large. Contrary to this assumption, we have shown here that this method works also well for relatively low laser field intensities and small values of n . A further result of the application of the saddle-point method leads to the conclusion that the x-ray spectra are mainly determined by those processes in which the x-ray photon is absorbed first. In this case, the atom gets ionized and the electron moves in the laser field. If its energy is small enough when it comes close to the atomic core, it can be recaptured and an x-ray photon is emitted. We have shown that this process is the most probable when the number of the exchanged photons satisfies the condition (31), $n\hbar\omega = I_0 - \hbar\omega_{\mathbf{K}}$. For $\hbar\omega_{\mathbf{K}} > I_0$, photons are emitted into the laser field, and the energy of the scattered x

ray $\hbar\omega_{\mathbf{K}'} = \hbar\omega_{\mathbf{K}} + n\hbar\omega$ is thus smaller than the energy of the incident one.

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