X-ray absorption by atoms under intense laser fields

P. Kálmán
Department of Experimental Physics, Physical Institute, Technical University of Budapest, H-1521 Budapest, Budafoki ut 8.F.I.I./10., Hungary
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The x-ray-absorption cross section in atoms both without and under intense laser fields is recalculated on the basis of gauge-invariance requirements in the first-order Born approximation. Better approximations of the intense-field-assisted x-ray-absorption cross section are also proposed.

I. INTRODUCTION

The x-ray absorption in atoms in the presence of an intense laser field has been considered by several authors.[1,2] In most of these papers perturbation calculus in the radiation gauge was used and generally not correctly applied. Because of this the traditional, first-order Born approximation without a laser frequently used by textbooks[3,4] also fails. The incorrect use of the perturbation calculus led to incorrect formulas for the S-matrix element, the transition probability per unit time, and the cross section. Therefore one of our aims is to rediscuss the process without this problem and in a gauge-invariant manner.

It is a well-known fact that measurable physical quantities, such as the transition probability per unit time and the corresponding cross section, cannot depend on the choice of the gauge of electromagnetic potentials. The problem is discussed in recent articles[5,6] from the point of view of the perturbation calculus of matter-field interactions in atomic physics and quantum optics. We use the terminology and the results of Refs. 5 and 6 throughout; furthermore, we restrict ourselves to the dipole approximation.

In order to make the problem and the situation clear first we summarize the steps of the traditional calculus of x-ray absorption in the first-order Born approximation without the presence of the laser field[4] (Sec. II). Then we repeat this train of thought bearing in mind the requirement of gauge invariance. We will see that the gauge-invariant, first-order Born approximation calculus of the x-ray-absorption cross section leads to different formulas from the ones commonly used.[3,4] The differences are discussed briefly (Sec. III). As a next step, the laser-assisted x-ray absorption is reconsidered also in the first-order Born approximation and taking into account gauge invariance. The results are briefly compared to that of Refs. 1 and 2 (Sec. IV). Finally, better approximations are proposed, which take into account the coexistence of the Coulomb and the laser field during the x-ray absorption (Secs. V and VI).

II. TRADITIONAL TREATMENT OF X-RAY ABSORPTION WITHOUT A LASER FIELD IN THE FIRST-ORDER BORN APPROXIMATION

First we repeat the usual treatment of the problem of x-ray absorption in atoms without the presence of the intense radiation field and in the first-order Born approximation.[4] We consider here one-electron processes only, and we restrict ourselves to hydrogenlike systems.

The initial state has the form

$$\psi_i(\mathbf{r},t)=u_i(\mathbf{r})e^{-iE_b t/\hbar}\ , \tag{1a}$$

with

$$u_i(\mathbf{r})=(\pi a^3)^{-1/2}\exp(-r/a)\ , \tag{1b}$$

where $\mathbf{r}$ and $E_b=-Z^2e^2/2a_0$ are the position vector and the binding energy of the electron, respectively, and $a=a_0/Z$ with a_0 being the Bohr radius and Z the nuclear charge of the atom. We restrict our discussion to the case of the hydrogenlike 1s state.

The final state is a free plane wave

$$\psi_f=\exp[i/\hbar(\mathbf{p}\cdot\mathbf{r}-Et)]\ , \tag{2}$$

where $\mathbf{p}$ and E are the momentum and energy of the outcoming electron, respectively.

The perturbation causing transition between these states is

$$H'=-(e/mc)\,\mathbf{A}_x(t)\cdot\mathbf{p}\ . \tag{3}$$

Here $\mathbf{p}=-i\hbar\nabla$ is the momentum operator and $\mathbf{A}_x(t)$ is the vector potential describing the x-ray radiation of a state of linear polarization and of frequency ω_x,

$$\mathbf{A}_x(t)=\mathbf{A}_{x0}\cos(\omega_x t),\quad \mathbf{A}_{x0}=A_{x0}\hat{\mathbf{e}}_x\ , \tag{4}$$

where $\hat{\mathbf{e}}_x$ is the unit vector parallel to the direction of polarization. We are now in the radiation gauge.

Substituting Eqs. (1)–(4) into the usual expression of the S-matrix element

$$S_{fi}=-i/\hbar\int dt\int d^3r\,\psi_f^*H'\psi_i\ , \tag{5}$$

one can obtain after integration by parts

$$S_{fi}=(eA_{x0}/mc)i\mathbf{p}\cdot(\hat{\mathbf{e}}_x/\hbar^2)U_i(\mathbf{p})\pi \times\delta(p^2/2m-E_b-\hbar\omega_x)\ , \tag{6}$$

where the definition of the momentum-space wave function

$$U_i(\mathbf{p})=\int\exp(-i\mathbf{p}\cdot\mathbf{r}/\hbar)u_i(\mathbf{r})d^3r \tag{7}$$

and the part of $\mathbf{A}_x(t)$ describing absorption, i.e.,

$A_{x0}\exp(-i\omega_x t)/2$,

were used. Substituting the momentum-space wave function of the hydrogenic 1s state[4]

$$U_i(\mathbf{p})=\frac{\pi^{1/2}2^3a^{3/2}}{[1+(pa/\hbar)^2]^2} \quad (8)$$

into Eq. (6), multiplying the result by the usual phase-space factor $d^3p/(2\pi\hbar)^3$ and the initial-state density, which is 2 in our case on the K shell, dividing it by the incident flux of x-ray photons $I_x/\hbar\omega_x$ (where $I_x=cE_{x0}^2/8\pi$ is the incident x-ray intensity with E_{x0}, the amplitude of the electric field strength, $=(c/\omega_x)A_{x0}$), and carrying out integrations, we obtain the total x-ray-absorption cross section of the K shell

$$\sigma=\frac{8\pi 2^5e^2(ap/\hbar)^3}{3mc\omega_x[1+(ap/\hbar)^2]^4} , \quad (9)$$

where $ap/\hbar=[(\hbar\omega_x-|E_b|)/|E_b|]^{1/2}$. In the $\hbar\omega_x \gg |E_b|$ limit Eq. (9) has the asymptotic form[3,4]

$$\sigma=2^{5/2}(8\pi/3)r_0^2\alpha^4Z^5(mc^2/\hbar\omega_x)^{7/2} , \quad (10)$$

where $r_0=e^2/mc^2$ is the classical electron radius and α is the fine-structure constant.

III. GAUGE-INVARIANT CROSS SECTION

Now we repeat the above calculation fulfilling the requirement of gauge invariance. As we know from Refs. 5 and 6 we have to use the noninteracting bound-state wave function for the initial state and $-e\mathbf{r}\cdot\mathbf{E}$ instead of Eq. (3) for the perturbation operator in the S matrix in the radiation gauge. Thus

$$\psi_i=e^{ie\mathbf{r}\cdot\mathbf{A}/\hbar c}u_i(\mathbf{r})e^{-iE_bt/\hbar} \quad (11)$$

and

$$H'(\mathbf{r},t)=-e\mathbf{r}\cdot\mathbf{E}(t) . \quad (12)$$

The state given by (11) has a gauge-independent energy eigenvalue E_b of the energy operator.[5,6] The function $u_i(\mathbf{r})$ is an eigenfunction of the unperturbed Hamiltonian $H_0=\mathbf{p}^2/2m+V(\mathbf{r})$, which is not a physical quantity.[5,6] The final state remains the same as given by Eq. (2).

Thus the correct S-matrix element of x-ray absorption in the radiation gauge and in the first-order Born approximation reads

$$S_{fi}=-i/\hbar\int dt\int d^3r\,\psi_f^*[-e\mathbf{r}\cdot\mathbf{E}(t)]\psi_i , \quad (13)$$

where ψ_i is given by Eq. (11) and ψ_f is a plane wave [Eq. (2)]. Using the definition of the momentum-space wave function $U_i(\mathbf{P}(t))$ given by Eq. (7) but with

$$\mathbf{P}(t)=\mathbf{p}-e\,\mathbf{A}(t)/c \quad (14)$$

and the relation determining the electric field vector $\mathbf{E}(t)$,

$$\mathbf{E}(t)=-\frac{\partial}{c\,\partial t}\mathbf{A}(t) , \quad (15)$$

one can obtain

$$S_{fi}=-\int \exp[i(E-E_b)t/\hbar]\frac{\partial}{\partial t}U_i(\mathbf{P}(t))dt . \quad (16)$$

The momentum-space wave function of the 1s state of a hydrogenlike system is given by Eq. (8) and so the time derivative of $U_{100}(\mathbf{P}(t))$ can be written as

$$\frac{\partial}{\partial t}U_{100}(\mathbf{P}(t))=\frac{\pi^{1/2}2^5a^{7/2}e\mathbf{p}\cdot\mathbf{E}(t)}{(v^2+1)^3\hbar^2} , \quad (17)$$

with $v=a|\mathbf{P}(t)|/\hbar$. Substituting this expression into Eq. (16) and using the $eA/c \ll p$ approximation we obtain

$$S_{fi}=\frac{\pi^{3/2}2^5a^{7/2}epE_{x0}(\hat{\mathbf{e}}_p\cdot\hat{\mathbf{e}}_x)}{i[1+(pa/\hbar)^2]^3\hbar^2}\delta((E-E_b)/\hbar-\omega_x) . \quad (18)$$

The corresponding total cross section is

$$\sigma=\frac{8\pi}{3}\frac{2^9(pa/\hbar)^3e^2\omega_xa^4m}{[1+(pa/\hbar)^2]^6\hbar^2c} , \quad (19)$$

which has the asymptotic form

$$\sigma=2^{9/2}(8\pi/3)r_0^2Z^5\alpha^4(mc^2/\hbar\omega_x)^{7/2} \quad (20)$$

in the $\hbar\omega_x \gg |E_b|$ limit. If we compare Eqs. (10) and (20) we can see that the only difference between the traditionally used and the gauge-invariant total cross sections is a factor of 4 in the high-energy limit, but in this limit the x-ray photon energy dependence of the cross section is the same in both cases. Usually the x-ray photon energy dependence of the cross section calculated in the first-order Born approximation is compared to the photon energy dependence of the measured cross sections, but because of the approximate character of a calculation of this type the magnitude of the cross section and therefore the presence or absence of the factor 4 was not essential.[3,4] That formula, which also gives the photoabsorption cross section near the absorption edge[7] and is referred to most frequently,[3,4] was computed correctly and in the xE gauge.

IV. LASER-ASSISTED X-RAY-ABSORPTION CROSS SECTION IN THE FIRST-ORDER BORN APPROXIMATION

The authors in Ref. 2 compute the S-matrix element, which governs the laser-assisted x-ray photoeffect, in the radiation gauge but they substitute for the initial electronic state the ground-state wave function Eqs. (1a) and (1b) of the unperturbed Hamiltonian $H_0=\mathbf{p}^2/2m+V(\mathbf{r})$ instead of the noninteracting bound-state wave function,[5] which has the form given by Eq. (11) in the laser field, where now $\mathbf{A}(t)$ is the vector potential, which describes the intense radiation (laser) field and the x-ray radiation together.

The use of the interaction Hamiltonian H' of the form given by Eq. (3) (which was used in Ref. 2) as perturbation operator in S-matrix calculus is also mistaken. It can be shown[5,6] that the operator $H'(\mathbf{r},t)$ given by Eq. (12) plays the role of perturbation in both (radiation and electric field) gauges and it has to be used in S-matrix element calculations. Thus the correct S-matrix element of laser-assisted x-ray absorption in the radiation gauge is of the form of Eq. (13) with ψ_i given by Eq. (11) and ψ_f a Volkov-type solution,

$$\psi_f = \exp\left[i/\hbar \left[\mathbf{p}\cdot\mathbf{r} - \int_0^t [\mathbf{p} - e\,\mathbf{A}(t')/c]^2/2m\, dt' \right] \right] , \tag{21}$$

where

$$\mathbf{A}(t) = \mathbf{A}_L(t) + \mathbf{A}_x(t) , \tag{22}$$

and $\mathbf{A}_L(t)$ and $\mathbf{A}_x(t)$ are the vector potentials of laser and x-ray radiation, respectively. So we can recognize that the factor $\exp[ie\mathbf{r}\cdot\mathbf{A}(t)/\hbar c]$ is also missing from the expression of S_{fi} of Ref. 2. It can easily be shown that Eq. (13) fulfills the gauge-invariance requirement. It is worth mentioning that Eq. (13) contains terms which give multiphoton ionization without x-ray absorption, but they make a very small contribution to the transition probability in the case of a strongly bound, inner-shell electron.

We suppose that the laser radiation and the x-ray field are described by linearly polarized classical beams which have states of polarization $\hat{\mathbf{e}}_3$ and $\hat{\mathbf{e}}_x$, respectively. Thus

$$\mathbf{A}_L(t) = \mathbf{A}_{L0}\cos\omega t = A_{L0}\hat{\mathbf{e}}_3\cos\omega t \tag{23}$$

and $\mathbf{A}_x(t)$ is given by Eq. (4). In this case the final state (21) has the form

$$\psi_f = \exp[i(\mathbf{r}\cdot\mathbf{p} - \hat{E}t)/\hbar] f_{\text{pol}}(\mathbf{p},t) , \tag{24}$$

with

$$\hat{E} = \mathbf{p}^2/2m + e^2(A_{L0}^2 + A_{x0}^2)/4mc^2 \tag{25}$$

and

$$f_{\text{pol}} = \exp\frac{i}{\hbar}\left[\frac{e\mathbf{p}}{mc}\left[\mathbf{A}_{L0}\frac{\sin\omega t}{\omega} + \mathbf{A}_{x0}\frac{\sin\omega_x t}{\omega_x} \right] - \frac{e^2A_{L0}^2\sin(2\omega t)}{8mc^2\omega} - \frac{e^2A_{x0}^2\sin(2\omega_x t)}{8mc^2\omega_x} + \frac{e^2A_{L0}A_{x0}}{2mc^2}\left[\frac{\sin(\omega_x-\omega)t}{\omega_x-\omega} + \frac{\sin(\omega_x+\omega)t}{\omega_x+\omega} \right] \right] . \tag{26}$$

The index "pol" indicates that the function f_{pol} depends on the state of polarization of the applied radiation fields. Substituting this final state into Eq. (13) and using the definition Eq. (7) of the momentum-space wave function with Eqs. (11), (14), (15), (22), and (16) one obtains

$$S_{fi}^{(1)} = -\int \exp[i(\hat{E}-E_b)t/\hbar] f_{\text{pol}}^*(\mathbf{p},t) \times \frac{\partial}{\partial t} U_i(\mathbf{P}(t))dt . \tag{27}$$

Here the upper index (1) refers to the first-order Born approximation. The time derivative of the momentum-space wave function of the 1s state of a hydrogenlike system in the $eA/c \ll p$ approximation is

$$\frac{\partial}{\partial t}U_{100} = \pi^{1/2}2^5a^{7/2}\hbar^{-2}e(\mathbf{p}\cdot\mathbf{E} - e\,\mathbf{A}\cdot\mathbf{E}/c) \times [1+(pa/\hbar)^2]^{-3} . \tag{28}$$

Now we select the terms from Eqs. (27) and (28) which correspond to laser-assisted x-ray absorption. A detailed examination of the order of magnitude shows that if $\hbar\omega_x > 1$ keV then in the case of laser intensities available nowadays those terms in f_{pol} and $\hat{E}$ [Eqs. (25) and (26)] which contain A_{x0} can be neglected; furthermore, only the terms $\mathbf{p}\cdot\mathbf{E}_x - e\,\mathbf{A}_L\cdot\mathbf{E}_x/c$ remain in Eq. (28). Here

$$\mathbf{E}_x = E_{x0}\hat{\mathbf{e}}_x \sin\omega_x t ,$$

which describes the electric field originating from the x-ray radiation and we use

$$\mathbf{E}_L = E_{L0}\hat{\mathbf{e}}_3 \sin\omega t$$

for the electric field generated by the intense laser. Using the Jacobi-Anger[8] formulas, the definition of the generalized Bessel functions $J_M(b,d)$ (Ref. 9) in f_{pol}, and the

$$-\exp(-i\omega_x t)/2i$$

part of $\sin(\omega_x t)$ we obtain for the S-matrix element of laser-assisted x-ray absorption

$$S_{fi}^{(1)} = \frac{\pi^{3/2}2^5a^{7/2}epE_{x0}}{i[1+(pa/\hbar)^2]^3\hbar^2}\sum_{M=-\infty}^{\infty} J_M(b,d)\left[\hat{\mathbf{e}}_p\cdot\hat{\mathbf{e}}_x\delta(\Delta/\hbar - M\omega) - \hat{\mathbf{e}}_3\cdot\hat{\mathbf{e}}_x\frac{eE_{L0}}{2p\omega}\{\delta[\Delta/\hbar-(M-1)\omega] + \delta[\Delta/\hbar-(M+1)\omega]\} \right], \tag{29}$$

and for the differential transition probability per unit time,

$$\frac{d^2W^{(1)}}{dE\,d\cos\theta_p} = \frac{2^7a^7e^2E_{x0}^2mp^3}{[1+(pa/\hbar)^2]^6\hbar^6}\sum_{M=-\infty}^{\infty}\{(\hat{\mathbf{e}}_p\cdot\hat{\mathbf{e}}_x)^2J_M(b,d)^2 - \frac{eE_{L0}}{2p\omega}(\hat{\mathbf{e}}_p\cdot\hat{\mathbf{e}}_3)(\hat{\mathbf{e}}_x\cdot\hat{\mathbf{e}}_3) \times [J_M(b,d)J_{M-1}(b,d) + J_M(b,d)J_{M+1}(b,d)]\} \times \delta(\Delta - \hbar M\omega) . \tag{30}$$

Here $\Delta=\hat{E}+|E_b|-\hbar\omega_x$, $\hat{\mathbf{e}}_p$ is the unit vector parallel to $\mathbf{p}$, m is the rest mass of the electron, $\hat{\mathbf{e}}_p\cdot\hat{\mathbf{e}}_3=\cos\theta_p$,

$$b=\frac{eE_{L0}p\cos\theta_p}{m\omega^2\hbar},\quad d=-\frac{e^2E_{L0}^2}{8m\omega^3\hbar}, \tag{31}$$

and the term proportional to $(eE_{L0}/2p\omega)^2$ was neglected.

The differential cross section can be obtained from Eq. (30) by dividing it by the x-ray photon flux $cE_{x0}^2/(8\pi\hbar\omega_x)$ and supposing states of parallel polarization for the laser and the x-ray fields,

$$\frac{d^2\sigma^{(1)}}{dE\,d\cos\theta_p}=\frac{8\pi 2^8(ap/\hbar)^3e^2\omega_x a^4 m}{[1+(pa/\hbar)^2]^6\hbar^2 c}\sum_{M=-\infty}^{\infty}\{(\hat{\mathbf{e}}_p\cdot\hat{\mathbf{e}}_3)^2J_M(b,d)^2-\frac{eE_{L0}}{2p\omega}\hat{\mathbf{e}}_p\cdot\hat{\mathbf{e}}_3 \times[J_M(b,d)J_{M-1}(b,d)+J_M(b,d)J_{M+1}(b,d)]\} \times\delta(\Delta-M\hbar\omega), \tag{32}$$

which leads to Eq. (19) in the laser-free case.

Our gauge-independent result is obviously different from that of Ref. 2. Moreover, in the case of moderately high laser intensities ($b\gg1$ and $|d|\ll1$, i.e., with $\hbar\omega=1.18$ eV this is true if $I_L<10^{13}$ W/cm^2) the term proportional to $(eE_{L0}/2p\omega)$ can be neglected and $J_M(b,d)=J_M(b)$ holds. Thus Eq. (32) becomes much simpler in this case. Our calculation is valid if $\hbar\omega_x\gg|E_b|$ because the first-order Born approximation can be used under this condition.

The results of the other articles dealing with laser-assisted x-ray absorption[1] are more or less in error, as they had been computed before the gauge problem was clarified[5,6] and thus they contain problems similar to the ones discussed at the beginning of this section.

V. THE *S*-MATRIX ELEMENT OF LASER-ASSISTED X-RAY ABSORPTION IN THE SECOND-ORDER BORN APPROXIMATION

Now we treat the problem in second order. We use the results of Reiss[9] where the *S*-matrix formalism with two potentials was worked out. In our case the applied two potentials are the radiation (laser plus x-ray) field and the Coulomb potential of the nucleus. In the preceding sections we considered first-order processes in the radiation field and the effect of the Coulomb potential on the outcoming electron was totally neglected. Now the scattering of the electrons, which are described by Volkov-type states, on the Coulomb potential will be taken into account. The corresponding *S*-matrix element[9]

$$S_{fi}^{(2)}=(i/\hbar)^2\int\psi_f^*(\mathbf{R},t_2)V(\mathbf{R})\Theta(t_2-t_1)\int d^3k\,\psi_k(\mathbf{R},t_2)\psi_k^*(\mathbf{r},t_1)[-e\mathbf{r}\cdot\mathbf{E}(t_1)]\psi_i(\mathbf{r},t_1)d^3R\,d^3r\,dt_2dt_1, \tag{33}$$

where $V(\mathbf{R})$ is the Coulomb potential felt by the electron, $\mathbf{R}$ and $\mathbf{r}$ are the electron coordinates, t_1 and t_2 the two time variables, $\Theta(t_2-t_1)$ is the Θ (or step) function, and $\psi_k(\mathbf{R},t_2)$ and $\psi_k^*(\mathbf{r},t_1)$ are solutions of the Volkovian type given by Eq. (21) with $\hbar\mathbf{k}$ standing for the momentum of the electron in the intermediate state with $\mathbf{k}$ the wave-number vector in this state. Introducing the Fourier transform $V(\mathbf{q})$ of the Coulomb potential,

$$V(\mathbf{q})=\int V(\mathbf{R})\exp(-i\mathbf{q}\cdot\mathbf{R})d^3R, \tag{34}$$

with the definition

$$\mathbf{q}=\mathbf{p}/\hbar-\mathbf{k} \tag{35}$$

($\mathbf{p}$ is the momentum of the electron in the final state), and using the equality

$$\int\psi_k^*(\mathbf{r},t_1)[-e\mathbf{r}\cdot\mathbf{E}(t_1)]\psi_i(\mathbf{r},t_1)d^3r=(\hbar/i)f_{\rm pol}^*(\mathbf{k},t_1)e^{i(\hat{E}_k-E_i)t_1/\hbar}\partial/\partial t_1U_i(\mathbf{K}(t_1)), \tag{36}$$

$\mathbf{K}=\mathbf{k}-e\,\mathbf{A}(t_1)/\hbar c$ in the momentum-space wave function [Eq. (7)] and the Jacobi-Anger formulas[8] in $f_{\rm pol}$, the second-order *S*-matrix element can be written as

$$S_{fi}^{(2)}=i/\hbar\int dt_1\int dt_2\int d^3k\,V(\mathbf{q})\sum_{N,M=-\infty}^{\infty}J_N(z)J_M(b_k,d)\Theta(t_2-t_1)e^{i[(E_f-E_k)/\hbar-N\omega]t_2}\partial/\partial t_1U_i(\mathbf{K}(t_1)) \times e^{i[(\hat{E}_k-E_i)/\hbar-M\omega]t_1}, \tag{37}$$

where $J_N(z)$ and $J_M(b_k,d)$ denote ordinary[8] and generalized[9] Bessel functions with arguments

$$z=(e\,\mathbf{A}_{L0}\cdot\mathbf{q}/mc\omega),\quad b_k=(eE_{L0}k\cos\theta_k/m\omega^2),\quad \cos\theta_k=\hat{\mathbf{e}}_k\cdot\hat{\mathbf{e}}_3, \tag{38}$$

$\hat{\mathbf{e}}_k$ is the unit vector parallel to $\mathbf{k}$, $E_f=p^2/2m$, $E_i\equiv E_b$, $E_k=h^2k^2/2m$, and $\hat{E}_k=E_k+e^2A_{L0}^2/4mc^2$. The time derivative of the initial-state, momentum-space wave function can be obtained from Eq. (28) using $\hbar\mathbf{K}$ instead of $\mathbf{P}$ in it. With the same approximations used in connection with Eq. (28),

$$\frac{\partial}{\partial t_1}U_i(\mathbf{K}(t_1))=\frac{i\pi^{1/2}2^4a^{7/2}eE_{x0}}{\hbar[1+(ka)^2]^3}\left[\mathbf{k}\cdot\hat{\mathbf{e}}_x e^{-i\omega_x t_1}-\frac{eE_{L0}}{2\hbar\omega}\mathbf{e}_L\cdot\mathbf{e}_x(e^{i(\omega-\omega_x)t_1}+e^{-i(\omega+\omega_x)t_1})\right] . \tag{39}$$

Substituting Eq. (39) into (37), supposing the adiabatic switching on and off for the x-ray, using the equality $V(q)=4\pi Z^2e^2/q^2$, and carrying out time integrations, we obtain

$$\begin{aligned}S_{fi}^{(2)}&=\pi^{5/2}2^7a^{7/2}Ze^3E_{x0}\hbar^{-2}\\&\times\int\frac{d^3k}{[1+(ka)^2]^3}\frac{1}{q^2}\sum_{N,M=-\infty}^{\infty}J_N(z)J_M(b_k,d)\left[\mathbf{k}\cdot\hat{\mathbf{e}}_x\delta(\omega_{fiNM}^{(0)})[-\pi\delta(\omega_{kiM}^{(0)})-iP/\omega_{kiM}^{(0)}]\right.\\&\qquad-\frac{eE_{L0}}{2\hbar\omega}\hat{\mathbf{e}}_L\cdot\hat{\mathbf{e}}_x\{\delta(\omega_{fiNM}^{(+)})[-\pi\delta(\omega_{kiM}^{(+)})-iP/\omega_{kiM}^{(+)}]\\&\qquad\left.+\delta(\omega_{fiNM}^{(-)})[-\pi\delta(\omega_{kiM}^{(-)})-iP/\omega_{kiM}^{(-)}]\}\right] ,\end{aligned} \tag{40}$$

with

$$\omega_{fiNM}^{(0,+,-)}=(E_f-E_i+\varepsilon)/\hbar-(N+M+s)\omega-\omega_x , \tag{41a}$$

$$\omega_{kiM}^{(0,+,-)}=(\hat{E}_k-E_i)/\hbar-(M+s)\omega-\omega_x , \tag{41b}$$

$\varepsilon=2\hbar\omega|d|$, and $q^{-2}=(p^2+k^2-2\mathbf{p}\cdot\mathbf{k})^{-1}$. Here P denotes principal value and $s=0,+1,-1$ correspond to upper indices $0,+,-$, respectively.

Now we show how one can obtain an approximate form of Eq. (40). In the case of moderately high laser intensities (for the conditions see the end of Sec. IV) the generalized Bessel function becomes equal to the ordinary one,[9] $J_M(b_k,d)=J_M(b_k)$, and the product of the two Bessel functions in Eq. (40) can be written approximately using the expression[10]

$$J_N(z)J_M(b_k)\approx(-1)^{N+M}J_{N+M}(z+b_k)\delta\left[N-(N+M)\frac{z}{z+b_k}\right] . \tag{42}$$

From Eqs. (31), (35), and (38), the $z=b-b_k$, and from the argument of the Dirac δ in (42), the relation

$$\cos\theta_k=\frac{M}{M+N}(p/\hbar k)\cos\theta_p \tag{43}$$

follows. Thus the integration in Eq. (40) over $\cos\theta_k$ can be carried out.

VI. THE S-MATRIX ELEMENT OF LASER-ASSISTED X-RAY ABSORPTION IN ANOTHER APPROXIMATION

The problem of finding approximate wave functions, which account for the influences of both (laser and Coulomb) fields on the final electron state, can be partially solved.[11] These solutions are used in recent multiphoton ionization calculations[12] giving results agreeing fairly well with experiments. Moreover, recently, a general method for the analytical evaluation of integrals occurring in bound-free transitions has been published,[13] which can also be used in laser-assisted x-ray transition calculations.

In view of the above facts the only modification that we have to make in the S-matrix element calculation as compared with Sec. IV is to use the above-mentioned approximate final state[11,12] of the form

$$\psi_f=U_f(\mathbf{p})\exp[i(\mathbf{p}\cdot\mathbf{r}-\hat{E}t)/\hbar]f_{\text{pol}}(\mathbf{p},t) , \tag{44}$$

with

$$U_f(\mathbf{p})=\exp(\pi\nu/2)\Gamma(1+i\nu)\times F(-i\nu,1,-i(pr+\mathbf{p}\cdot\mathbf{r})/\hbar) \tag{45}$$

in the S-matrix element, if we want to give another approximation for the laser-assisted x-ray absorption. Here $\nu=(pa/\hbar)^{-1}$, $\Gamma(x)$ and $F(a,b,c)$ denote the Γ and the hypergeometric functions, respectively. Thus the doubly differential transition rate and cross section can be written

$$\begin{aligned}d^2W/d\Omega\,dE&=\sum_{L=-\infty}^{\infty}(d^2W/d\Omega\,dE)_L ,\\d^2\sigma/d\Omega\,dE&=\sum_{L=-\infty}^{\infty}(d^2\sigma/d\Omega\,dE)_L ,\end{aligned} \tag{46}$$

where

$$(d^2W/d\Omega\,dE)_L=\frac{I_xa^2|T_L|^2\delta(\hat{E}_f-E_i-L\hbar\omega-h\omega_x)}{4\pi^2\alpha mc^2[1-\exp(-2\pi\nu)]} , \tag{47}$$

$$(d^2\sigma/d\Omega\,dE)_L=2(h\omega_x/I_x)(d^2W/d\Omega\,dE)_L , \tag{48}$$

with

$$T_L = \int_{-\pi}^{\pi} d\varphi\, f_L(\varphi) B(\mathbf{p}/\hbar, \mathbf{E}_{L0}\sin\varphi) , \tag{49}$$

$$B(\mathbf{p}/\hbar,\mathbf{E}_{L0}) = a^{-5/2} \int u_i(\mathbf{r}) \hat{\mathbf{e}}_3\cdot\mathbf{r} F[i\nu, 1, i(pr+\mathbf{p}\cdot\mathbf{r})/\hbar] \exp[-i(\mathbf{p}/\hbar + eE_{L0}\hat{\mathbf{e}}_3 \sin\varphi/\hbar)\cdot\mathbf{r}] d^3r , \tag{50}$$

and

$$f_L(\varphi) = \exp i(L\varphi - b\cos\varphi + d\sin 2\varphi) . \tag{51}$$

Integral (50) can be evaluated analytically by the aid of Eq. (6.9) of Ref. 13 and the expression (49) has to be integrated numerically.

VII. CONCLUSIONS

In this paper we briefly summarized the gauge-invariant method of computation of laser-free and laser-assisted x-ray-absorption cross sections and gave two different methods for obtaining an approximation one order higher than the traditionally used and incorrectly derived first-order Born expressions.

Our results can be used also near the absorption edge, which makes it possible to investigate theoretically a very exciting, combined process where the presence of the laser is essential. If the energy of the x-ray photon is less than the ionization potential on a given shell, but this energy defect is small compared to the energy of the laser photon, then the absorption can occur with the help of the laser radiation.[14]

If we assume that our formulas account well for these phenomena, a two-beam (laser plus x-ray) experiment can provide information on the amount of shielding of the laser radiation (near the nucleus) by the outer electrons.[15]

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