Time-dependent postcollision interaction effects in THz-field-assisted Auger decay.

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The effects of post-collision interaction (PCI) in the time-evolution of photoinduced Auger decay, assisted by terahertz (THz) field, is theoretically investigated. We propose a time-dependent model which is based on the quantum-mechanical description of the photoinduced Auger process and quasiclassical description of the PCI. The suggested model is used for calculating the PCI distortion of the Auger spectrum at different temporal overlap of the exciting extreme ultraviolet pulse and the streaking THz pulse.

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I. INTRODUCTION

The term Post-Collision Interaction (PCI) is used to describe the effects of the interaction of charged particles in the final state of the atomic collision process [1]. In particular in the photoinduced Auger process, PCI is the interaction between the photoelectron, the Auger electron and the residual ion [2, 3]. The PCI distorts the shape of the Auger line in the spectrum and shifts the position of its maximum. Furthermore, PCI is responsible for the recapture of slow photoelectrons back to the ion. The effects of PCI were widely discussed in experimental [4–9] and theoretical [10–18] works in the 80's and 90's. With the advent of free-electron lasers (FEL) in the extreme ultraviolet (XUV) and X-ray regions, and of new XUV sources based on high harmonic generation (HHG) producing ultra-short XUV pulses, the experimental investigation of the time evolution of the Auger decay has become possible [19–25]. Recently, the first time-resolved observation of the PCI effect in Auger decay has been reported [26]. In the experiment, the Auger spectra for the transitions MNN in Kr and NOO in Xe were investigated using a time-resolved pump-probe method. The Auger transitions were induced by ultra-short XUV pulses. The temporal variation of the Auger spectra were measured using a terahertz (THz)-field-driven streak camera. The difference in the dependence of the spectra on the time-delay between the XUV and THz pulses on the ascending and descending slopes of the streaking vector potential (an energetic chirp) has been revealed which was interpreted as the effect of PCI. For the interpretation of the results the analytical semiclassical approach, developed in ref. [27], was used.

The quantum mechanical description of the temporal evolution of the field-assisted Auger decay based on the solution of the time-dependent Schrödinger equation has been developed in the papers [18, 28]. However, the application of these approaches for the considered case of Auger transitions in the THz field is practically impossible at present, since the relevant numerical calculations would demand prohibitively long computer time.

In order to overcome this problem, S. Bauch and M. Bonitz [27] solved the relevant 1D Schrödinger equation and also used the Monte Carlo molecular dynamics method based on classical mechanics. They also developed an analytical (quasi) classical model which describes the PCI effects in the THz assisted Auger transition. The model is applicable at the extreme of the THz electric field (corresponding to zero values of the vector potential) where the electron does not acquire a net kinetic energy shift. Very recently this analytical model was used to predict the time-dependent PCI effect of the THz assisted Auger emission in noble gas atoms [29].

In the present work we suggest a more rigorous albeit simple quantum mechanical description of the PCI effects in the time-resolved Auger process. It is based on the time-dependent theory of the Auger process induced by an ultrashort XUV pulse in the presence of a powerful laser field as developed by A.K. Kazansky et al. [28]. In order to include PCI, we use the quasiclassical approach suggested in [13]. With this model we are able to investigate the variation of the PCI effect in the time evolution of the Auger spectra as a function of the overlap between the XUV and the THz pulses. Using the proposed model we calculated the spectra of Auger electrons for MNN transitions in Kr atoms which are most suitable for experimental investigation [29]. The results are compared to the analytical semiclassical model.

In the next section we describe the suggested model and the approximations used. Section 3 shows the results of calculations. Conclusions are presented in section 4.

II. BASIC EQUATIONS AND APPROXIMATIONS

A time-dependent theory of Auger decay induced by ultra-short XUV pulses in a strong laser field has been developed in [28]. It is based on solving a system of time-dependent Schrödinger equations which describes the photoionization of an inner atomic state and the decay of the created vacancy. In this approach the Auger

electron interacting with the strong laser field is treated in the strong field approximation [30]. Thus the theoretical description is appropriate for the comparatively fast Auger electrons with energies $E_A > 1$ a.u. In the cited paper [28] the following closed expression for the probability of Auger electron emission has been obtained for the near threshold photoionization, which predicts rather accurately the shape of the Auger electron spectra for short exciting pulses. In this work, atomic units are used unless otherwise indicated.

$$W(\vec{k}_A) = \frac{\Gamma}{8\pi} \left| \int_{t_0}^{\infty} dt e^{iQ(\vec{k}_A, t) - \frac{\Gamma}{2}(t-t_0)} \times \int_{t_0}^t dt' e^{i(E_e - i\frac{\Gamma}{2})(t'-t_0) - i(\omega_X + \epsilon_0)t'} \tilde{\mathcal{E}}_X(t') D_{\vec{k}_e} \right|^2, \quad (1)$$

where

$$Q(\vec{k}_A, t) = - \int_{t_0}^t \left[-E_A + \frac{1}{2} [\vec{k}_A - \vec{A}_L(t')]^2 \right] dt'. \quad (2)$$

Here $\vec{k}_A$ is the linear momentum of the emitted Auger electron, t_0 is the time when the XUV pulse starts, $\tilde{\mathcal{E}}_X(t')$ is the envelope of the XUV pulse, ω_X is its central frequency, E_e is the photoelectron kinetic energy, $E_e = k_e^2/2$, ϵ_0 is its binding energy in the atom, Γ is the Auger decay width, and $D_{\vec{k}_e}$ is the dipole matrix element characterizing the interaction of the electron with the electromagnetic field of the XUV pulse. The value $Q(\vec{k}_A, t)$ is the phase, related to the Volkov phase [31], accumulated by the Auger electron moving in the THz field which is characterized by the vector potential $\vec{A}_L(t)$, E_A is the nominal energy of the Auger electron. In the derivation of Eq.(1) the interaction of the photoelectron with the THz field is ignored. Expression (1) describes the Auger electron spectrum for arbitrary XUV and THz pulses, both linearly polarized in the same direction. In the following, the matrix element $D_{\vec{k}_e}$ is set equal to unity. The latter assumption means that we ignore the energy dependence of the matrix elements. Thus we can apply this model in an energy interval which is much smaller than the typical energy of the considered Auger electrons. Within this model, only the shape of the Auger spectrum and energy shift can be discussed but not the absolute value of the cross section.

In the above approach both photoelectron and Auger electron are considered as independent and non-interacting. Therefore the PCI effects are not included. In order to take them into account, we use the semiclassical approach as described in Ref. [13]. The main part of the PCI is considered to be induced by the change of the screening of the ionic core, which is felt by both electrons when the fast Auger electron overtakes the slower photoelectron. This change of the screening leads to an increase of the energy of the Auger electron and correspondingly to a decrease of the photoelectron's energy. If one denotes the total energy gained by the Auger electron in post-collision interaction as $S_A(t)$, then the

outgoing Auger electron will be observed at an energy $E = E' + S_A(t)$ where

$$E' = k_A^2/2 = E - S_A(t) \quad (3)$$

denotes the energy of the electron ignoring PCI.

In the semiclassical approach the term $S_A(t)$ may be calculated as $S_A(t) = 1/r^*(t)$ where r^* is the distance from the ion nucleus to the point where Auger electron overtakes the photoelectron. With sufficient accuracy it is given as [12] (see also [27])

$$r^* = tp_r + \delta r^* \quad (4)$$

with $p_r = k_A k_e / (k_A - k_e + A_L(t_0) - A_L(t))$. The value δr^* is a small correction depending on the radii of the initial and the final electron sub-shells involved [27]:

$$\delta r^* = \frac{(k_A - A_L(t))R_e - (k_e - A_L(t_0))R_A - A_L(t)(R_A - R_e)}{k_A - k_e + A_L(t_0) - A_L(t)}. \quad (5)$$

Here $A_L(t) = |\vec{A}_L(t)|$, $k_A = |\vec{k}_A|$, R_A and R_e are the radii of the initial subshells of the Auger and the photoelectron, respectively.

Note that the energy gain $S_A(t)$ depends on the emission time of the Auger electron. At larger t , the Auger electron overtakes the photoelectron at a larger distance from the nucleus, and therefore the energy gain by the Auger electron, is smaller.

We further assume that the Auger electron is detected along the polarisation direction. Taking into account that $E_e \approx \omega_X + \epsilon_0$ we obtain from Eq. (1) the final expression

$$W(E) = \frac{\Gamma}{8\pi} \left| \int_{t_0}^{\infty} dt e^{iQ(E, t) - \frac{\Gamma}{2}(t-t_0)} \int_{t_0}^t dt' e^{\frac{\Gamma}{2}(t'-t_0)} \tilde{\mathcal{E}}_X(t') \right|^2 \quad (6)$$

with the phase

$$Q(E, t) = - \int_{t_0}^t [-E_A + E - S_A(t') \mp k_A A_L(t') + A_L^2(t')/2] dt', \quad (7)$$

where the minus (plus) sign corresponds to the detection of Auger electron in (opposite) the direction of the vector potential.

This expression reduces to that obtained by A. Russek and W. Mehlhorn [13] if we take $A_L(t) = 0$ and assume that the XUV pulse is very short (delta-function). On the other side, if we ignore the $S_A(t)$ term, we return to the Eq. (1) which describes the Auger electron spectrum induced by a short XUV pulse.

III. RESULTS AND DISCUSSION

In this section we show some results of the calculations using the theoretical model introduced above, which illustrates the PCI effect for different conditions. In particular, we compare the influence of PCI to the streaking effect in the presence of a THz field. In all calculations

FIG. 1. Vector potential of the THz field in atomic units (black solid curve) and the XUV pulses (in arbitrary units) used in the calculations as a function of time in fs. The position of the maximum of the X-ray pulse for several delay times used in the calculations is indicated by numbers. The dashed line shows the corresponding THz electric field in atomic units multiplied by 10^4 .

we use the model THz vector potential described by the analytical expression

$$A_L(t) = A_0 \exp(-t^2/2\sigma_L^2) \cos(2\pi t/T_L), \quad (8)$$

$$-0.75 T_L < t < 0.75 T_L.$$

Here A_0 and T_L are the amplitude and period of the THz field vector potential. This vector potential is similar to the vector potential of the single-cycle THz field used in experiments [32]. The ionizing XUV pulse is described by a Gaussian envelope of electric field:

$$\tilde{\mathcal{E}}_X(t) = \exp(-(t - t_d)^2/2\sigma_X^2), \quad (9)$$

with intensity FWHM = $2\sqrt{\ln 2}\sigma_X$ and a time-delay t_d with respect to the maximum of $A_L(t)$. Fig. 1 shows the used vector potential with amplitude $A_0 = 0.29$ a.u., $\sigma_L = 475$ fs and period $T_L = 1900$ fs which corresponds to a THz field with the central frequency of 0.53 THz and a field strength of 120 kV/cm. In the same figure we show the relative positions of six different Gaussian XUV pulses of 10 fs duration (FWHM). The position 1 corresponds to the zero crossing of the vector potential, while positions 2-6 are located on the decreasing slope of it.¹

As target atom we have chosen Kr and considered the MNN Auger transitions which are well investigated experimentally [33, 34]. In particular, we have chosen the

FIG. 2. The shape of the Auger line calculated with (solid curves) and without (dashed curves) PCI effect for different pulse duration (FWHM) of the exciting XUV pulse: 5 fs (lines 1), 10 fs (lines 2), 20 fs (lines 3). The excess energy is 0.5 eV. The spectral lines are normalized to unity in the maximum, the energy scale is relative to the nominal Auger electron energy, E_A .

transition $M_5N_1N_{2,3}(^1P_1)$ resulting in an Auger electron at an energy of 37.7 eV [34]. The corresponding radii of the orbits were taken from Hartree-Fock calculations to be $R_e = 0.538$ a.u. and $R_A = 1.952$ a.u. The threshold energy for Kr ($3d_{5/2}$) ionization is 93.8 eV [35]. The Auger lifetime for this transition is $\tau = 7.5$ fs, $\Gamma = 88$ meV [36]. As is shown in [29], the Kr MNN Auger transition is a good candidate for future experimental investigations of the PCI effects in Auger decays.

A. Auger line shape distorted by PCI in absence of THz field

Let us first consider the PCI effects in the Auger process generated by a short XUV pulse in the absence of the THz field ($A_L(t) = 0$). As it is well known, PCI affects the shape of the Auger spectral line and the position of its maximum. In Fig. 2 we show the shape of the line in the Auger spectrum calculated using expression (6) with and without PCI effect for different XUV pulse durations of 5 fs, 10 fs and 20 fs for the excess energy 0.5 eV (energy of the photoelectron). In earlier calculations of PCI effect for Auger transitions (see [13] and references therein), a prompt ionization was assumed, which corresponds to an ultrashort XUV pulse $\tau_{XUV} \rightarrow 0$. In contrast, Figure 2 shows that the shape of the Auger line depends on the duration of the XUV pulse. The width of the lines for non-zero τ_{XUV} is determined not only by the Auger width but also by the energy spread of the ionizing pulse. When the PCI effect is ignored, the maximum of the Auger line is at the nominal energy of

¹ Note that our definition of vector potential differs by sign from that used in Ref. [27]. Therefore, also the terms "rising slope" and "falling slope" of the vector potential are interchanged.

FIG. 3. The shape of the Auger line calculated taking into account the PCI effect for an XUV pulse duration of 5 fs and different excess energies 0.5 eV (line 1), 1.5 eV (line 2), 2.5 eV (line 3), and 10 eV (line 4). The spectral lines are normalized to unity in the maxima, the energy scale is relative to the nominal Auger electron energy, E_A . The inner figure shows the absolute energy shift of the peak of each Auger line as a function of the excess energy E_e . The dashed line is used to guide the eyes.

the Auger electron. Its width diminishes by increasing the pulse duration. The PCI shifts the maximum and changes the shape of the line. By increasing the XUV pulse duration, the relative influence of the PCI diminishes. Furthermore, the energy shift becomes smaller and the line shape approaches a Gaussian shape which is determined by the Gaussian shape of the XUV pulse. If the pulse (Eq. 9) is not Gaussian, the Auger line shape will depend on the XUV pulse shape.

In Fig. 3 we show the calculated Auger line shapes for one duration of the exciting XUV pulse (5 fs), but for different excess energies (kinetic energy of photoelectron) of 0.5 eV, 2.5 eV, 5 eV and 10 eV. In accordance with [13], the maximum distortion and maximum energy shift occur at smaller excess energy (see inner figure). By increasing the excess energy the shift decreases and the line shape becomes close to a Lorentzian shape.

B. Influence of THz field on Auger line shape including PCI

When the THz field is switched on, the Auger spectrum is modified by the streaking effect and this effect strongly depends on the time delay between the THz and the XUV pulses. In Fig. 4 we compare the spectra for one and the same XUV pulse duration (10 fs) and one value of excess energy (1 eV) but for different time delays as shown in Fig. 1. Note that the spectra presented in Fig. 4 are not normalized. They are shown in arbitrary units but

FIG. 4. Spectra of the Auger decay in the THz field calculated including the PCI effect (solid lines) and without PCI (dashed lines) for an XUV pulse duration of 10 fs, for an excess energy of 1 eV and for different time delays between the XUV and the THz field. The numbers near the peaks indicate the XUV pulse position as shown in Fig. 1. Panel (a) Auger electrons detected in forward direction, panel (b) Auger electrons detected in the backward direction.

the units are the same for all spectra. The shown spectra are calculated taking the PCI effect into account (solid lines) and ignoring the PCI effect (dashed lines). The presence of only the THz field shifts the position of the Auger line and changes its width. In addition the PCI effect distorts and shifts the spectral line as well. Both, the streaking and PCI, change the width of the Auger line which makes the observation of the PCI effect and its quantitative investigation even more complicated.

In the experiment [26], the shapes of the lines in spectra of Auger electrons streaked by the THz field have been studied for opposite directions of Auger electron emission: along the polarization of both XUV and THz fields and opposite to it. This is equivalent to study the streaking at the descending and at the ascending slopes

of the vector potential. In Fig. 4(a) we present the results of the calculations for the emission angle $\theta = 0$, i.e. along the polarization, while Fig. 4(b) shows the results for $\theta = \pi$. The spectrum 1 corresponds to the XUV pulse position close to zero vector potential (see Fig. 1). The maximum of the Auger line is close to the nominal position and the line is broadened. The spectra 2 to 6 show a large energy shift due to interaction with the THz field. On the descending slope of the vector potential, the Auger electron peak in the forward direction is shifted to higher energies and becomes broader. In the backward direction, the peak is shifted to smaller energies and becomes narrower. In both cases, the PCI effect shifts the peak to higher energies and makes it broader.

It is interesting to discuss the variation of the peak widths as a function of the time delay in more detail. Since the spectra presented in Fig. 4 are calculated for the same transition but for different time delays, they only differ by the interaction with the THz field. Thus, the total number of emitted Auger electrons (the area under the peak) is the same, and a larger value in the maximum of the spectrum corresponds to a smaller width. Consider first the case without PCI (dashed curves) at Fig. 4(a). One sees that going from spectrum 1 to spectrum 6 (decreasing the time delay) the width of the line first increases and then starts to decrease. The widths of the spectra in Fig. 4(b) also show a similar behaviour. This modulation of the width due to streaking can be explained as follows. From the classical theory of streaking [32, 37], one knows that the width of the line acquired due to streaking is proportional to the time-derivative of the streaking THz vector potential, corresponding to the THz electric field. The latter is presented in Fig. 1 for the chosen vector potential as a dashed curve. The variation of the spectral widths in Fig. 4 follows the change of the derivative of the vector potential.

In paper [29], we suggested to characterize the influence of the PCI effects by the ratio of the Auger line widths for opposite emission directions $\theta = 0$ and $\theta = \pi$. It was shown that the ratio of the widths, which can be measured in an experiment, is sensitive to the PCI effect. In order to obtain such ratio we fitted the streaked Auger lines by the Gaussian curves and determined their width and the ratio. The resulting ratios are shown in Fig. 5 for different time-delays.

Qualitatively, the influence of the PCI on the streaked Auger line width and their ratio may be explained as follows. Considering expression (6) for the Auger line shape, the phase $Q(E, t)$ in the first integral is quickly varying. In order to approximately evaluate the integral one can use the saddle point approximation [37]. The saddle point is defined by the condition $\frac{\partial Q(E, t)}{\partial t}|_{t=t_s} = 0$ which gives the relation

$$-E_A + E - S_A(t_s) \mp k_A A_L(t_s) + A_L^2(t_s)/2 = 0. \quad (10)$$

Here minus (plus) sign corresponds to emission in forward (backward) direction. For the considered experiments,

FIG. 5. The ratio of the widths of the Auger line calculated for emission in forward and backward directions as a function of delay. The points in the solid curve (upper line) were calculated with PCI, the points in the dashed curve (lower line) without PCI. The parameters of the pulses are the same as in Fig. 4. The lines are drawn to guide the eyes.

$k_A \gg A_L(t)$. Solving the above equation, we find

$$k_A = \sqrt{2[E_A + S_A(t_s)]} \pm A_L(t_s). \quad (11)$$

Eq. (10) links the final momentum k_A , and hence the final Auger electron energy $E = \frac{k_A^2}{2}$, with the time of the Auger electron emission t_s . It qualitatively explains the evolution of the Auger spectral line with the time delay. Going from the delay point 1 to point 6, the vector potential increases, thus the Auger energy on the right slope (plus sign in (11)) also increases while on the left slope decreases. Using Eq. (11) one can also estimate the width of the spectral line for different delays:

$$\delta E = k_A \delta k_A \approx k_A |dA_L(t_s)/dt \pm E_A^{-1/2} dS_A(t_s)/dt| \delta t. \quad (12)$$

If one ignores PCI ($S_A(t) = 0$), then the width is determined by the derivative of vector potential. It is increasing (modulus) by changing the delay from position 1 to 6. Besides, k_A is also changing with the time-delay. The ratio of widths in forward and backward direction is

$$\delta E_+ / \delta E_- = \frac{\sqrt{2E_A} + A_L(t_s)}{\sqrt{2E_A} - A_L(t_s)} \approx 1 + 2 \frac{A_L(t_s)}{\sqrt{2E_A}}. \quad (13)$$

The ratio is increasing going from point 1 to point 6 (see dashed curve in Fig. 5).

When PCI is taken into account it gives a contribution to the widths. As we already discussed, the energy gain $S_A(t)$ diminishes with t , thus the derivative $dS_A(t)/dt$ is negative. On the right slope (forward emission, plus sign in Eq. (12)) the derivative of the vector potential is negative, therefore both terms in Eq. (12) have the same sign, the width is increasing due to PCI. On the

FIG. 6. (a) The shape of the Auger line in the THz field calculated taking into account the PCI effect for the XUV pulse close to the zero crossing of vector potential (position 1 in Fig. 1), for three different THz frequencies 0.53 THz (solid line), 1.05 THz (dotted line) and 2.1 THz (dashed line). An XUV pulse duration of 10 fs, excess energy of 0.5 eV, and THz field strength of 120 kV/cm have been used in the calculations. Panel (b) shows the same as in (a) but for the time delay corresponding to position 5 in Fig. 1.

contrary, on the left slope (minus sign in Eq. (12)), the PCI diminishes the width of the line. The resulting ratio, shown in Fig. 5 by the solid curve increases steeper from delay 1 to delay 6 than the dashed curve calculated without PCI.

The above calculations have been done for the THz field strength 120 kV/cm and frequency 0.53 THz. In order to investigate the influence of the PCI on the line shape at different frequencies of the streaking field, we made calculations for the same field strengths but varying the frequencies. The results are shown in Fig. 6. We remind that in the analytical semiclassical model suggested in [27], the streaked Auger spectrum does not depend on THz frequency. Indeed, the spectrum is considered when the XUV pulse is set at zero vector potential. Then the main parameter which determines the influence of the

THz field is the time-derivative of the vector potential which is actually the THz electric field. Thus, according to the semiclassical model, for the fixed strength of the THz field, the results should not depend on the frequency. We have verified this prediction using our model. The results are shown in Fig. 6(a). The calculations made for 0.53 THz, 1.05 THz and 2.1 THz give almost identical results for both the shape and the position of the maximum. Naturally, at other delays the vector potential is non-zero and therefore the position of the Auger spectral line depends on the delay while the width is determined not only by the PCI, but also by the streaking. Since the vector potential scales as E_L/ω_L for a fixed THz field strength, it depends on the frequency. Therefore, the line shape and position depend on the frequency as well, as shown in Fig. 6(b).

C. Comparison of the quantum and analytical semiclassical models

Finally, we compare the results of the calculations made using the suggested model, based on the quantum-mechanical approach, with the results of the analytical semiclassical model [27, 29]. We remind that in the latter model, simple analytical expressions for the spectral line shape for an infinitesimal XUV pulse duration have been suggested [27]. For a positive derivative of the streaking electric field $\dot{A}_L > 0$, the spectral line shape $f_+(\epsilon)$ is presented as:

$$f_+(\epsilon) = \Gamma_4 \frac{k_+ - \epsilon_-}{k_+} e^{-\Gamma_4(k_+ - \epsilon_+)}, \quad (14)$$

where $\Gamma_4 = |\alpha|\Gamma$ with $\alpha = (2k_A\dot{A}_L)^{-1}$. For negative values of $\dot{A}_L < 0$, the spectral line shape is:

$$f_-(\epsilon) = 2\Gamma_4 e^{-\Gamma_4\epsilon_+} \left(\frac{\epsilon_-}{k_-} \cosh \Gamma_4 k_- - \sinh \Gamma_4 k_- \right). \quad (15)$$

In these equations $k_{\pm} = \sqrt{\epsilon_{\pm}^2 \pm |\beta|}$, $\epsilon_{\pm} = \epsilon \pm \frac{\beta}{4}\delta r^*$ with $\beta = 4k_A\dot{A}_L/p_r$. In order to obtain the Auger spectrum for a finite pulse duration τ_X , one convolutes these spectral line shapes with the streaked energy spectrum $f_X(\hat{\epsilon})$ due to the finite XUV pulse duration:

$$W(E) = \int_{-\infty}^{+\infty} d\hat{\epsilon} f_X(\hat{\epsilon}) f_{\pm}(E - \hat{\epsilon}). \quad (16)$$

Here $f_X(\hat{\epsilon}) = (\sqrt{\pi}\Gamma_X)^{-1} \exp(-\hat{\epsilon}^2/\Gamma_X^2)$, with $\Gamma_X = k_A\dot{A}_L\tau_X$. For a more detailed description of the semiclassical analytical model the reader is referred to S. Bauch and M. Bonitz paper [27].

As a typical example, in Fig. 7 we show the dependence of the Auger line widths for the emission in forward and backward directions on the energy ratio of photo and Auger electrons for the case of an XUV pulse duration of 5 fs and an excess energy of 1 eV at a THz field of

FIG. 7. The widths of the Auger line calculated for the emission in the forward (solid lines) and the backward (dashed lines) directions as a function of the ratio of the excess and Auger electron energies. The calculations have been performed for the zero crossing point of the THz vector potential. The result of the calculations using the present quantum mechanical model are shown as black lines, the results of the analytical semiclassical model of ref. [29] are shown as red lines (lighter gray). The calculations have been done for an XUV pulse duration of 5 fs, for an excess energy of 1 eV and THz field strength of 60 kV/cm.

60 kV/cm. The calculations using the quantum model have been performed for a time delay close to the zero-crossing of vector potential where the analytical model is valid. The classical analytical model predicts much broader lines and a considerably larger difference between widths as compared to the quantum model (larger PCI effect).

We note that both models use approximations, which are however significantly different. In the analytical model [27], the time-to-energy mapping is calculated using a classical description of the Auger electron motion. The energy gained by the Auger electron, due to the change of screening when it overtakes the photoelectron, is added to its classical energy. In the present quantum model the Auger decay is described quantum mechanically where the energy gain is added to the phase of the

Auger electron. Furthermore, the method of averaging over the XUV pulse duration is significantly different for the two models. In the quantum model we consider, in accordance with the rules of quantum mechanics, the amplitude of the Auger emission induced by the finite XUV pulse is calculated, which is then squared to obtain the probability. In contrast, in the analytical model [27], the probability of the Auger emission is calculated for an infinitesimally short XUV pulse, which is then convoluted with the spectral distribution of the finite pulse. The latter approach corresponds to the so-called ad hoc model, based on the rate equations. (See discussion, for example, in [38, 39]). Therefore it is not surprising that the calculated Auger widths are different in the two models.

IV. CONCLUSION

We presented a theoretical model which combines a fully quantum mechanical description of the time-dependent Auger process induced by an ultra-short XUV pulse in the presence of a THz field, with the quasiclassical description of PCI. The model enables the investigation of the time evolution of PCI effects experienced by Auger electrons in a THz field. We analysed the dependence of the PCI distorted Auger spectra on the pulse duration of the exciting XUV pulse as well as the effect of PCI on spectra of Auger electrons in the presence of a THz field. An advantage of the suggested model is that it can be used for any time delay between the exciting XUV and probing THz pulses. The quantum mechanical results are compared to the results of an analytical (semi) classical model [27]. We show that the latter model predicts considerably larger PCI effects in THz streaking spectra as compared to the present quantum model. Further theoretical efforts as well as new experiments devoted to the investigation of the time evolution of PCI effects would be very desirable.

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