Time-resolved Spectroscopy of Interparticle Coulombic Decay Processes

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We report theory for time-resolved spectator resonant Interparticle Coulombic Decay (ICD) processes. Following excitation by a short XUV pulse, the spectrum of the resonant ICD electron develops. Strong-field ionization quenches the decay at different time delays and initiates regular ICD, whose ICD electron signal can be measured without interference effects. The typical lifetimes of ICD processes allow for the observation of oscillations of the time- and energy-differential ionization probability. We propose to utilize this oscillation to measure lifetimes of electronic decay processes.

Interparticle Coulombic Decay (ICD) [1, 2] is an electronic decay process of ionized systems consisting of at least two weakly bonded units, be it atoms, molecules or clusters. ICD has been observed in multiple systems like noble gas clusters [3–6] and clusters of different solvent molecules like water [7, 8] or ammonia [9, 10]. It allowed to explain the repair mechanism of the enzyme photolyase [11] and was used to establish a more efficient double ionization strategy [12]. ICD is furthermore discussed as a source of slow electrons, which are most efficient in damaging the DNA after exposure to high energy radiation or radioactive materials in the human body [14–19]. In this work, we shed light on this fundamental process by offering a time-resolved perspective directly of the electron dynamics.

Due to developments in creating short pulses in the extreme ultraviolet (XUV) and x-ray domain [21] a time-dependent investigation of ICD processes is feasible. Fano profiles of a much faster autoionization (AI) process were recently measured [22, 23]. A few time-resolved investigations of ICD have already been performed theoretically and experimentally, where the ions produced in the process were measured [24, 31]. However, electrons can be measured with higher energy resolution than ions and grant direct access to the electron dynamics and interference during the process. In this work, we will therefore focus on the time evolution of the time- and energy-differential ionization probability, propose how it can be measured in experiment, and discuss how decay lifetimes can be determined from the time-resolved signal.

In brief, the ICD process starts from a unit \( A \), which is ionized in the inner valence shell. This vacancy is filled by an electron from the same unit and the excess energy is simultaneously transferred to a neighbouring unit \( B \). The latter is consequently ionized by emission of the ICD electron. The two positively charged units undergo a Coulomb explosion (see Fig. 1). A related process is initiated by an excitation of unit \( A \). This resonant ICD (RICD) can be characterized by the behaviour of the excited electron: it either participates in the decay process or not. The respective processes are called participator RICD (pRICD) [32] and spectator RICD (sRICD) [32–37]. In this work, we will focus on the sRICD signal: Unit \( A \) is excited from the inner valence. The vacancy is then filled by an electron from the valence and the excess energy is used to ionize the neighbouring unit \( B \) (see Fig. 1). This process is usually characterized by lifetimes of several tens to hundreds of femtoseconds. After the sRICD process, the excited unit \( A \) decays via fluorescence within a few nanoseconds. AI and pRICD are competing decay channels and their effect on the sRICD signal is taken into account.

We propose to initiate a sRICD process by exciting with a short extreme ultraviolet (XUV) pulse. The system will then decay under emission of an sRICD electron. This is illustrated in Fig. 1 for the case of the neon dimer after an excitation to the \( \text{Ne} \ 2s^{-1}5p \) state. At a later time \( t_s \), a second short and intense infrared (IR) laser pulse quenches the sRICD process by ionization. By varying the time delay \( t_s \) one should be able to observe the time-dependent formation of the sRICD signal similar to the AI process measured in Ref. [22]. The spectrum includes an oscillation in both the kinetic energy of the emitted electron as shown in Fig. 1(a) and in time. At the same time, the proposed quenching would initiate an ICD process involving the excited ion \( A^{\ast\ast} \). Due to the strong field ionization initiating the process, the well-separated signal would be interference free and therefore show a Lorentzian lineshape [Fig. 1(c)]. In this Paper we provide the basic formulation for a purely electronic solution upon which more complex scenarios, including nuclear dynamics, will be built in future work.

The relevant property for the description of the time evolution of the ICD processes is the time- and energy-differential ionization probability obtained from the time-dependent wavefunction \( \Psi(t) \) by

\[
P(E_{\text{kin}}, t) = \sum_i \langle |E_i| \Psi(t) \rangle^2.
\]

Here \( |E_i| \) denotes a continuum state with energy \( E_i \), which entails both the kinetic energy \( E_{\text{kin}} \) of the emitted electron and the energy of the final cationic state \( i \). These continuum states are orthogonal to all bound states of the system and amongst each other. Because the signals of the competing decay channels do not overlap, we can and will focus on the sRICD signal.

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FIG. 1. Illustration [20] of the considered process. At $t = 0$, a spectator Resonant Interparticle Coulombic Decay (sRICD) is initiated by XUV excitation. At a later time $t_s$, which in this example is 35 fs, a second strong infrared laser pulse quenches the sRICD process by ionization and thereby initiates ICD. The signals of the respective electrons with kinetic energies $E_{\text{kin}}$ are well separated. While the sRICD appears from the start of the XUV pulse centered at $t = 0$, the ICD signal appears after the second pulse. This approach allows for a time-resolved measurement of the sRICD signal and an interference free measurement of the ICD signal.

sRICD: Unit $A$ is excited from the inner valence shell. The created vacancy is filled with an electron from the outer valence and the excess energy is simultaneously transferred to $B$, which emits the sRICD electron.

ICD: The initial state is created by removing the excited electron in $A$. It is then filled by an electron of the outer valence of $A$ while the excess energy is transferred to $B$, which consequently emits the ICD electron. The two units are both positively charged and therefore undergo Coulomb explosion. Spectrum: The sRICD signal centered around 5.3 eV before the second pulse shows the buildup of a Fano profile, with an additional oscillation in energy $\cos[(E_{\text{kin}} + E_{\text{fin}} - E_r)t]$ (see (a) and text). After depopulation of the sRICD resonant state around $t_s$, only the direct term of Eq. (3) with a Gaussian shape remains (see (b)). For the ICD signal centered around 0.6 eV shown in (c), only the resonant term of Eq. (3) contributes, which has a Lorentzian shape.

Atomic units are used throughout unless stated otherwise.

We obtain the wavefunction of the system by solving the time-dependent Schrödinger equation $i\partial_t |\Psi(t)\rangle = H(t) |\Psi(t)\rangle$ for a model system consisting of the ground state $|G\rangle$, the resonant state $|R\rangle$ for the sRICD and the resonant state $|I\rangle$ for the ICD process, as well as two sets of continuum states characterized by the respective final state energy of the decay process. All parameters describing a general resonant state are designated by the index $r$. The Hamiltonian consists of the single configuration Hamiltonian $H_0$, the residual configuration interaction operators $V_{\text{RICD}}$ and $V_{\text{ICD}}$, and the operator $H_X(t)$ of the exciting XUV pulse:

$$H(t) = H_0 + V_{\text{RICD}} + V_{\text{ICD}} + H_X(t).$$

(1)

The effect of the ionizing infrared pulse is modelled by terminating the sRICD and starting the ICD process at the time of the second pulse $t_s$. We will come back to this point below.

The continuum state of the sRICD can couple to other continuum states under emission of a photon. This process is usually several orders of magnitudes slower than the electronic decay process and is therefore ignored in this work. We assume low field strengths of the XUV pulse and therefore use first order perturbation theory to describe its interaction with the system. Hence, the wavefunction evolves according to

$$|\Psi(t)\rangle = \tilde{U}(t, t_0) |G(t_0)\rangle - i \int_{t_0}^t dt' \tilde{U}(t, t') H_X(t') |G(t')\rangle.$$  

(2)

Here, $\tilde{U}(t, t_0)$ is the time evolution operator from a time $t_0$ until time $t$ of the unperturbed system pertaining to
the first three terms on the right hand side of Eq. (1).

We are free to choose an energy reference and therefore

\[ \langle E_{SR}|\Psi(t)\rangle = -i \int_{t_0}^{t} dt' \langle E_{SR}|U_0(t,t')H_X(t')|G\rangle - \int_{t_0}^{t} dt' \int_{t'}^{t} dt'' \langle E_{SR}|U_0(t,t'')|E_{SR}\rangle V_{ER} \langle R|U_R^{\prime}\rangle(t'',t') \langle R|H_X(t')|G\rangle \]

\[ - \int_{t_0}^{t} dt' \int_{t'}^{t} dt'' \int_{t'}^{t} dE'_{SR} \langle E_{SR}|U_0(t,t'')|E_{SR}\rangle V_{ER} \langle R|U_R^{\prime}\rangle(t'',t') \langle E'_{SR}|H_X(t')|G\rangle \]

\[ - \int_{t_0}^{t} dt' \int_{t'}^{t} dt'' \int_{t'}^{t} dE_o' \langle E_o'|U_0(t,t'')|E_{SR}\rangle V_{ER} \langle R|U_R^{\prime}\rangle(t'',t') \langle E_o'|H_X(t')|G\rangle. \tag{3} \]

In these expressions, \( U_0(t,t') \) is the free particle time evolution operator. \( V_{ER} = \langle E|V|R\rangle = \sqrt{\Gamma_{SR}/(2\pi)} \) is related to the partial sRICD decay rate of the resonant state \( \Gamma_{SR} \) and \( U_R^{\prime}\rangle(t'',t') \) is the Fano time evolution operator, which is specific to the resonant state \( |R\rangle \). The variables of the other, competing, processes are designated with the index \( o \). The total decay width of the RICD resonant state is given by \( \Gamma_R = \Gamma_{SR} + \Gamma_o \). For a derivation and explicit expressions of the four amplitudes in Eq. (3), see the Supplementary Material [38].

The first term of Eq. (3) describes the direct excitation and ionization to the continuum state, while the second term describes the excitation from the ground state to the resonant state followed by a decay to the continuum state. The third, indirect, term describes the direct excitation and ionization to the continuum state related to the sRICD final state, which couples to the resonant state, which then again decays into the continuum state. The last term is similar to the indirect term, but couples to the continuum of the competing pRICD and AI channels. The interference of these different terms leads to the characteristic Fano profile [39].

In our model system, where the nuclei are kept fixed, we evaluated Eq. (3), see [38], and simulated the time-dependent build up of the Fano resonance for the sRICD process for parameters corresponding to those of the neon dimer at the equilibrium distance of 3.08 Å [40] after an excitation to the Ne2s\(^{-1}\)2p\(^6\)5p\(_2\) state, which we show in Table I. All simulations were performed with ELDEST [41] [42] using the parameters specified in [38] and choosing the Fano parameter \( q = 10 \). The exact \( q \) value is unknown to us, but we expect it to be larger than unity due to the low probability for direct single photon ionization and excitation. We have performed calculations for a range of \( q \) parameters and the main conclusions remain unchanged [38].

We choose a Gaussian XUV pulse shape, and describe the interaction in the length gauge and dipole approximation such that \( H_X(t') = -E_X(t')\mu \) with \( \mu \) the dipole operator and \( E_X(t') = -\partial_{t'}\{A_0X \cos(\Omega t')\exp[-t'^2/(2\sigma_X^2)]\} \), where \( \sigma_X = n_x\pi/\Omega \sqrt{\ln 2} \). The exciting pulse for the results in Fig. 1 has \( A_0X = 5 \times 10^8 \) W/cm\(^2\), \( \Omega = 47.6930 \) eV, and a FWHM = 6.1 fs corresponding to 50 cycles. This duration ensures that the bandwidth is so small that only the Ne2s\(^{-1}\)2p\(^6\)5p\(_2\) state is resonantly excited.

We assumed a complete population transfer from the resonant state of the sRICD process to the resonant state of the ICD process during the second ionizing pulse over a time of 15 fs as realized experimentally[22]. For this we assumed a Gaussian shaped change in the population of either of the two resonant states and that the ICD signal is unaffected by pulse shape effects [38]. Since we assume a direct population of the resonant state of the ICD process \( |I\rangle \) from the resonant state of the sRICD process \( |R\rangle \) with a short and intense laser pulse, we assume, that the terms of Eq. (3), which are mediated by the continuum, can be neglected. After the end of the ionizing pulse the amplitude of the ICD process associated with resonance \( |I\rangle \) therefore reads

| TABLE I. Energies and lifetimes for the excited states Ne2s\(^{-1}\)2p\(^6\)np - Ne (n = 4, 5) undergoing RICD. The resonant energies are taken from Ref. [? ], the final state energies of the sRICD Ne2s\(^2\)2p\(^5\)(P\(_3/2,1/2\)) np - Ne2p\(^3\)l(P\(_3/2,1/2\)) of the pRICD and Al Ne2s\(^2\)2p\(^5\)(P\(_3/2,1/2\)) - Ne and the ICD process were averaged to give approximations of non-relativistic energies. The lifetimes, \( \tau \), of the sRICD and pRICD + AI are from Ref. [35] and the ICD lifetime are from Ref. [? ]. |
|-------------|--------|--------|--------|
| n            | 4      | 5      |
| E\(_r\) [eV] | 47.1230| 47.6930| 48.4750|
| E\(_{fin}\) [eV] | 41.8391| 42.4138| 21.6290| 47.8688|
| \( \tau(2s^{-1}(np_x)^3\Sigma_u^+) \) [fs] | 112    | 106    | 206    | 98    |
\[ \langle E | \Psi(t) \rangle = -\int_{t_0}^{t} \int_{t_s + \delta t}^{t} dt'' \langle E | U_0(t, t'') | E \rangle V_{EI} \langle I | U_I^R(t'', t_s) | I \rangle \sqrt{N_0}, \]  

\[ P(E_{\text{kin}}) \propto \exp[-\sigma^2(E_{\text{kin}} + E_{\text{fin}} - \Omega)^2] \]  

\[ \cos[(E_r - E_{\text{kin}} - E_{\text{fin}})\tau] \exp(-\frac{\Gamma_r}{2} t), \]  

where \( N_0 \) is the population in \( | R \) at \( t_s - \delta t \), with \( \delta t \) being half the duration of the infrared pulse \[38\]. Equation \[4\] shows that the ICD channel is populated without any interference, and we therefore obtain a pure Lorentzian profile in Fig. 1(c). After the second pulse, the resonant state of the sRICD process is totally depopulated. Therefore, only the direct term contributes to the signal yielding a Gaussian as shown in Fig. 1(b).

In the investigation of decay processes with short laser pulses, the shortness comes with the cost of an energy broadening. As a consequence, the kinetic energy spectrum of an sRICD electron is given by a Fano profile centered around the kinetic energy, that corresponds to the energy of the resonant state, convoluted with a Gaussian centered around the kinetic energy, that would correspond to a direct excitation and ionization into the final state \[38\]. Here, we show the Voigt profile part inherent to all terms.

The shape of the spectra are illustrated for different numbers of cycles \( n_X \) for the exciting pulse in Fig. 2. There, the mean pulse energy was chosen to be on resonance and therefore, the Fano profile is centered on the maximum of the Gaussian. It is clearly seen, how the peak is narrowed with an increased number of laser cycles in the exciting pulse. In order to only excite into a single state we choose \( n_X = 50 \), such that other excited states are outside \( 3\sigma_E \) of the energy distribution of the exciting pulse. In future investigations of the interaction between several decaying resonant states, a smaller number of cycles will be appropriate.

For the case of an off-resonant excitation, the Fano profile and the Gaussian will not be centered around the same kinetic energy of the sRICD electron and the sRICD electron peak will be damped accordingly as illustrated by the dashed line of Fig. 2 for \( n_X = 30 \).

It can be shown analytically that, in addition to the overall structure at infinite times, the sRICD and ICD spectra show an oscillation in both energy and time, which is proportional to \[38\]

\[ \cos[(E_r - E_{\text{kin}} - E_{\text{fin}})\tau] \exp(-\frac{\Gamma_r}{2} t), \]  

where \( r = R, I \). The variation in energy, illustrated in Fig. 1(a), is in agreement with Ref. \[46\]. As can be seen from Eq. \[6\], the oscillation is also visible in time as shown in Fig. 3 for a fixed kinetic energy of the sRICD electron of \( E_{\text{kin}} = 5.3 \) eV.

Such an oscillation requires long enough lifetimes of the resonant state. The comparably slow sRICD process offers the opportunity to observe and utilize it. It has recently been observed experimentally for the first time.
for an AI process [47]. In both the latter and in our case, a discrepancy between the actual and the fitted lifetime is observed. Given the analytical expressions of this work, we are able to understand this discrepancy. The kinetic energy in Fig. 3 is slightly higher than the kinetic energy corresponding to the resonant state. The further away from the resonance this energy is chosen, the shorter the period of this oscillation. The oscillation is exponentially damped by the lifetime of the decaying state. However, long lifetimes, such as the ICD processes, this oscillation allows for a new way of measuring the lifetime of the underlying processes. Moreover, the basic formulation opens the door for future investigations in controlling the decay processes and to guide time-resolved experimental studies.

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