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Reply to "Comment on 'Dynamics of transfer ionization in fast ion-atom collisions' "

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In the Comment, it is claimed that the so-called electron-electron-Auger mechanism of transfer ionization, proposed in Voitkiv *et al.* [Phys. Rev. Lett. **101**, 223201 (2008)] and Voitkiv [J. Phys. B **41**, 195201 (2008)], does not exist. In the Reply, we argue against this claim.

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(I) Let us start the Reply with remarks concerning some well-known processes resulting in the capture of an electron by an ion when the ion collides with free electrons or atoms and the place of the electron-electron-Auger (EEA) mechanism (questioned in the Comment) among these processes.

(a) Suppose that a beam of fast ions penetrates a gas consisting of free electrons. When an ion collides with an electron, electron-ion recombination can occur. Viewing the ion-electron collision in the rest frame of the ion, we can easily see that one of ways to recombine is represented by the so-called radiative recombination. In this process, an electron incident on an ion forms a bound state with the ion via the interaction with the radiation field resulting in the emission of a photon carrying away the energy difference between the initial and the final electron states.

If the electron gas is dense enough such that there is a large probability to find two electrons in the vicinity of the ion, then another recombination process becomes effective. In this process, which is often called three-body recombination, one of these two electrons forms a bound state with the ion via the interaction with the other electron which takes the energy excess.

Both radiative and three-body recombinations are well-known processes.

(b) Suppose now that a beam of fast ions penetrates a gas which consists of neutral atoms instead of free electrons. In such a case, an analog to electron-ion recombination in collisions with free electrons will be electron transfer in which an ion captures an electron initially bound in an atom.

Although atomic electrons are bound, in collision processes where the change in their momenta is much larger than the typical electron momentum in the initial atomic state, they behave as quasifree (for instance, in radiative electron capture [1], in binary-encounter emission [2], in excitation of highly charged ions by collisions with atoms [3,4], in correlated radiative double-electron capture [5–7], etc.).

Electron transfer proceeding via emission of a photon is called radiative electron capture. When this process occurs in fast collisions in which the change in the electron momentum is comparatively very large, the atomic electron to be transferred behaves during the collision as quasifree, whereas, the atomic nucleus (the atomic core) is merely a spectator. This radiative electron capture is analogous to radiative recombination and is very often treated as radiative recombination [1] with averaging the corresponding cross section over the Compton profile of the atomic electron.

It was pointed out by us [8,9] that, in fast ion-atom collisions, an analog of three-body recombination is also possible: One of the atomic electrons is transferred to the ion via the interaction with another atomic electron, whereas, the nucleus of the atom is just a spectator during the process. This other electron gets a large recoil and, as a result, is emitted from the atom. One of the signatures of this three-body recombination process, which we call the EEA [10], is the emission of electrons with large velocities in the direction opposite to the motion of the ion.

The simplest (rather rough) theoretical estimate of this process can be given using the transition amplitude where the initial state is the (undistorted) atomic state and the final state describes one electron captured by the ion and the other electron emitted. The interaction resulting in the transition is the electron-electron interaction.

(II) The authors of the Comment claim that the EEA, in fact, does not exist because it does not follow from the consideration which uses the Oppenheimer-Brinkman-Kramers (OBK) (OBK-like) transition amplitude given in its prior and post forms by formulas (4a) and (4b) of the Comment.

However, the use of the amplitudes (4a) and (4b) is a rather weak starting point for questioning the EEA since they possess a number of severe shortcomings: In particular, these amplitudes are strongly gauge dependent violating charge conservation, yield large unphysical contributions, do not give good results even for a much simpler case of electron capture in a three-body system consisting of an electron and two nuclei (and even in the limit of asymptotically high collision velocities for this simple capture), etc.

One should also note that the point that the OBK approximation does not predict the EEA is, in fact, not new. Indeed, using the amplitude (4b), transfer ionization was theoretically considered several years ago in Ref. [11] (and the consequent papers), and no signature of the EEA was found. (The authors of the Comment also use the amplitude (4b) in their calculation repeating basically the same consideration.) Since it has been very well known for a long time (see, e.g., a review [12] and references therein) and is elementary to prove that the post and prior forms (4a) and (4b) of the OBK amplitude are equivalent [13], it is quite clear from the consideration of Ref. [11] that the EEA does not follow from the OBK approximation. When working on the results presented in Refs. [8,9], we were already well aware of this point but disregarded it because of the reasons which are mentioned in the previous paragraph and are considered below [14].

Let us, for instance, briefly discuss the last term (with V_{Np}) in the amplitude (4b) (this amplitude was used in the calculation presented in the Comment). In the Comment and in a recent paper [15] (where the theory part was performed by the first and fourth authors of the present Comment), it is claimed that this term yields an important contribution to transfer ionization in fast collisions. According to this term, the transfer ionization may proceed merely via the (single) interaction between the projectile and the nucleus of the atom.

However, in the transfer ionization, the typical recoil velocity of the atomic nucleus after the collision with the ion is orders of magnitude smaller than the orbiting velocities of the atomic electrons such that these electrons feel practically no change in the field of the nucleus of the atom. Then, if the projectile does not interact with the electrons and the field of the atomic nucleus acting on the electrons does not change, how do the electrons “know” that the collision has happened and what (which physical mechanism) does force them to make any transitions?

The answer to the above question is quite clear: There is no physical mechanism which might lead to transfer ionization (or to any electron transitions, in general) if only the interaction between the projectile and the nucleus of the target is involved (unless the momentum transfers are so huge that the nucleus of the atom is essentially kicked off the atom leaving the electrons, that is certainly not the case here). The fact that the amplitude (4b) [or (4a)] does suggest that such transfer ionization is possible is just a consequence of the fundamental shortcomings inherent to this type of amplitude where there is a direct transition between initial and final (asymptotic) states belonging to different Hamiltonians. (These shortcomings, of course, remain no matter how accurately one describes these states.)

It is actually very well known that, in fast ion-atom collisions with momentum transfers typical for atomic processes (ionization, excitation, electron transfer, projectile-electron excitation and loss, electron-positron pair production, etc.), the interaction between the ion and the atomic nucleus does not influence the electron (lepton) transitions. The physical reason for this is that this interaction practically does not change the motion of these heavy particles in the reaction zone.

Further, in a few lines before formula (11) of the Comment, the authors claim that, in the amplitude (4a), the effect of V_{12} is canceled by the term with V_{N1}, where V_{12} and V_{N1} are the electron-electron interaction and the interaction between the nucleus of the target and the electron to be captured, respectively [see formula (4a) of the Comment]. However, in fast collisions, the term with V_{12} where the target nucleus is not directly involved in the transition and is more or less just a spectator and the term with V_{N1} where the target nucleus heavily participates in the transfer and gets a recoil momentum which is much larger than the typical momenta in the atomic Compton profile, clearly describe different reaction pathways of transfer ionization. Therefore, based on these simple physical grounds, one cannot expect such a cancellation.

One more example worth mentioning here is a theoretical description of the correlated two-electron capture via emission of a single photon (this process is very closely related to the correlated transfer ionization, see Ref. [16]). If one uses amplitudes of types (4a) and (4b) for this process, then the calculated result for the total cross section exceeds by orders (!) of magnitude the upper limits for this cross section which were set experimentally (see, e.g., Fig. 2 of Ref. [17]). (Note that differential cross sections are, as a rule, much more sensitive to the approximations used than the total cross section.) The reason for this very strong disagreement is large unphysical contributions to the transition amplitude caused by the nonorthogonality of the initial and final electron states.

One should add that, when such amplitudes are used for the consideration of the “normal” radiative electron capture (in which one electron is captured via emission of a single photon), then the results may already be not very far from the reality (see, e.g., Fig. 1 of Ref. [17]) provided a proper gauge is chosen (see the first Born results in Fig. 1 of Ref. [18]). Thus, the actual difficulties inherent to the use of the amplitudes of types (4a) and (4b) sharply increase when one goes from transfer processes, in which only one electron actively participates, to a much more complicated case of transfer involving two active electrons.

The examples considered in this section clearly show that, when one attempts to treat a complicated four-body process of transfer ionization using such imperfect tools, such as the amplitudes (4a) and (4b), one has to be very careful in analyzing whether there is real physics behind the obtained result or it is just an artifact caused by the basic shortcomings inherent to such amplitudes. (Moreover, one must be very cautious even with those terms in these amplitudes, which could be interpreted as describing real physical mechanisms since these amplitudes, because of their obvious shortcomings, are not capable of yielding correct relationships between these mechanisms.)

(III) In our recent paper [16], we studied transfer ionization in collisions with fast highly charged ions. The correlated part of this process was considered using a treatment principally different from that employed in Refs. [8–10] and was based on the impulse approximation, which has been proven to be a very useful and powerful theoretical tool in considering capture processes (note that the impulse approximation yielded results for the correlated two-electron radiative capture not contradicting the experiment [6,17], whereas, the OBK-like approximation strongly failed [17]). Within this treatment, the initial and final states are built using eigenfunctions of the same Hamiltonian, and thus, the treatment does not have the shortcomings inherent to considerations based on the amplitudes (4a) and (4b).

According to the results of Ref. [16], the EEA mechanism does exist, surviving even in very strong fields generated by highly charged ions. It is also important that, in fast collisions with low charged ions, the treatment of Ref. [16] yields results for the EEA which are very close, both in shape and in absolute values, to those obtained using the treatment of Refs. [8–10].

Note that, in the paragraph after formula (9) of the Comment [as well as before formula (4a) and in a couple of other places], the authors seem to confuse the approach of Refs. [8–10] with that of Ref. [16].

(IV) In the paragraph after formula (9) of the Comment, the authors claim that we sum the contribution of the amplitude (9) with that of the OBK. In the same paragraph, they also criticize the introduction of the continuum-distorted-wave (CDW) distortion factor in Refs. [8–10] saying that this should lead to the appearance of the term with derivatives in the (residual) interaction.

The claim that we sum the contribution of the amplitude (9) with that of the OBK is not correct: We certainly do not do that.

The claim that the derivatives should always appear in the effective interaction is also not true. For instance, the term with derivatives does not appear in the CDW model of radiative electron capture [17–19]. Such a term is also absent in distorted-wave models of projectile-electron excitation and loss [20,21]. In Refs. [8–10], the term with derivatives does not appear because the distortion factor is related to the field of the incident projectile, whereas, the perturbation causing the transition is the electron-electron interaction.

In Refs. [8–10], the CDW distortion factor makes the initial and final states less nonorthogonal, strongly reducing the unphysical contributions to the transition amplitude. Besides, the introduction of this factor enables one to approximately account for the electron-electron-Thomas mechanism [22] of transfer ionization.

(V) In the Comment, the authors especially stress that they use an accurate trial function for approximating the ground state of helium. We have already remarked that the basic shortcomings inherent to the OBK amplitudes remain no matter how accurately one describes the initial and final states in these amplitudes. Besides, such functions are normally obtained by fitting the binding energy which does necessarily mean that the parts of the atomic wave function, most important for the transition matrix elements in question, are well reproduced by the trial function.

(VI) Experimental results on the spectra of the recoil ions and electrons produced in transfer ionization in fast collisions [23,24] strongly support the existence of the EEA mechanism.

The main results of the consideration given in this Reply can be briefly summarized as follows:

(1) The basic physics of the EEA mechanism is very simple and transparent. The EEA is analogous to three-body recombination; it also has similarities to radiative electron capture and is closely related to the highly correlated process of radiative double-electron capture.

(2) The critique of the existence of the EEA mechanism in the Comment is ungrounded because it is based on the application of the amplitudes which possess severe shortcomings.

(3) In Ref. [16], the correlated transfer ionization was considered using a treatment quite different from that of Refs. [8–10]. This treatment is based on the impulse approximation, is free of the shortcomings inherent to the OBK consideration given in the Comment, and it does confirm the existence of the EEA mechanism.

(4) Experimental results on transfer ionization in fast collisions also strongly support the existence of the EEA mechanism.

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