Transfer Ionization in Collisions with a Fast Highly Charged Ion

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Transfer ionization in fast collisions between a bare ion and an atom, in which one of the atomic electrons is captured by the ion whereas another one is emitted, crucially depends on dynamic electron-electron correlations. We show that in collisions with a highly charged ion a strong field of the ion has a very profound effect on the correlated channels of transfer ionization. In particular, this field weakens (strongly suppresses) electron emission into the direction opposite (perpendicular) to the motion of the ion. Instead, electron emission is redirected into those parts of the momentum space which are very weakly populated in fast collisions with low charged ions.

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Electron-electron interaction is responsible for very many phenomena studied by the different fields of physics ranging from astrophysics to biophysics. Amongst them atomic physics and its part—physics of ion-atom collisions—often deal with most basic and clear manifestations of this interaction.

Atomic excitation and ionization [1–4], projectile-electron excitation and loss [2,3,5], electron transfer (capture) [1,4], and pair production [1,4,5], belong to the elementary reactions occurring when a projectile ion collides with a target atom. A combination of these reactions in a single-collision event is also possible and in such a case the electron-electron interaction during the collision when the external field is rapidly changing (dynamic electron correlations) is often crucial.

In particular, mutual ionization in which both a target atom and a (partially stripped) projectile ion eject electrons, and transfer ionization in which one of atomic electrons is captured by a projectile ion whereas another one is emitted, represent processes where dynamic electron correlations play a crucial role [2,3,5–8].

Transfer ionization in fast collisions of low charged ions (mainly protons) with helium is attracting much attention [9–18]. This process can be analyzed in terms of different reaction mechanisms which are characterized by distinct features in the electron emission pattern. Depending on whether the electron-electron interaction plays in them a crucial role, these mechanisms can be termed ''correlated'' or ''uncorrelated.''

Uncorrelated mechanisms are independent transfer ionization (ITI) and capture–shake-off (C-SO). In ITI electron capture and emission occur due to ''independent'' interactions of the projectile with two target electrons. According to the C-SO, a capture of one atomic electron by the ion leads to a sudden change of the atomic potential for another electron resulting in its emission.

The correlated mechanisms include electron-electron Thomas (EET) and electron-electron Auger (EEA). Within the EET transfer ionization proceeds [7,19,20] via a binary collision of the projectile with one of atomic electrons and a consequent rescattering of this electron on another atomic electron. After these two collisions one of the electrons moves together with the projectile while the other is emitted perpendicular to the projectile motion.

The functioning of the EEA mechanism is based on the fact that merely the presence of the projectile makes the target unstable with respect to a kind of Auger decay. Indeed, viewing the collision in the rest frame of the projectile we can see that one of the electrons, bound initially in the atom, can make a transition into a bound state of the ion by transferring the energy excess to another atomic electron which, as a result of this, is emitted from the atom in the direction of the atomic motion [8,14]. In the rest frame of the atom the emitted electron moves opposite to the projectile velocity [8,14,16].

The mechanisms, mentioned above, were proposed for describing transfer ionization in collisions between a light atom and a low charged ion moving with a velocity v much higher than the typical velocities of the electron(s) in their initial and final bound states: $v \gg Z_a e^2/\hbar$ and $v \gg Z_i e^2/\hbar$, where $Z_a e$ and $Z_i e$ are the charges of the nuclei of the atom and ion, respectively.

What, however, can one say about transfer ionization in fast collisions with highly charged ions (HCIs) when the charge $Z_i e$ of the ion is so large that $Z_i \sim \hbar v/e^2$? One can expect that in such collisions, characterized by very strong fields generated by the HCI, not only cross sections for transfer ionization would be much larger than in collisions with equivelocity low-charged ions but also new interesting features could arise in this process.

Therefore, in this Letter we explore transfer ionization in fast collisions with HCIs. It will be seen that a strong field of the HCI has a drastic effect on the correlated transfer ionization: it weakens the EEA mechanism, eliminates the EET mechanism, and leads to qualitatively new structures in the emission spectrum. Atomic units ($\hbar = m_e = e = 1$) are used throughout except where otherwise stated.

Correlated transfer ionization.—We are mainly interested in the correlated transfer ionization and begin with its treatment. This treatment will be semiclassical in which only the electrons are described quantum mechanically whereas the nuclei of the ion and atom are considered classically. In fast collisions the trajectories of the nuclei are practically straight-line trajectories. It is convenient to use the rest frame of the ion and to take its position as the origin.

According to scattering theory the exact (semiclassical) transition amplitude can be written as

$$a_{\mathrm{fi}} = -i \int_{-\infty}^{+\infty} dt \langle \psi_f(t) | \hat{W}(t) | \Psi_i^{(+)}(t) \rangle. \quad (1)$$

Here $\Psi_i^{(+)}$ is an exact solution of the time-dependent Schrödinger equation with the full Hamiltonian $\hat{H}$ which describes two electrons moving in the external field of the nuclei and interacting with each other, ψ_f denotes the final state of the two electrons, and $\hat{W}$ is that part of $\hat{H}$ which is not included in the wave equation for ψ_f. Since the contribution to transfer ionization from collisions with spin-flip is negligible we disregard the spin parts of the states Ψ_i and ψ_f.

In the correlated transfer ionization the velocities of the electrons with respect to the nucleus of the atom in the final state are of the order of v [16]. Besides, in this state the relative velocity of the electrons as well as the velocity of the emitted electron with respect to the projectile are also of the same order. Therefore, when this process occurs in fast collisions with HCIs, for which one has $Z_i \sim v$ but $\max\{Z_a, 1\} \ll v$, the motion of both electrons in the final state ψ_f is driven by the field of the HCI whereas the other interactions can be neglected. Thus, we have

$$\psi_f(t) = \frac{1}{\sqrt{2}} \left(\chi_b(\mathbf{r}_1) \chi_{\mathbf{p}}^{(-)}(\mathbf{r}_2) \pm \chi_b(\mathbf{r}_2) \chi_{\mathbf{p}}^{(-)}(\mathbf{r}_1) \right) \times \exp[-i(\varepsilon_f + p^2/2)t], \quad (2)$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the coordinates of the electrons, χ_b is the bound state of an electron captured by the HCI with an energy ε_f, and $\chi_{\mathbf{p}}^{(-)}$ is the state of the emitted electron which moves in the HCI's field and has asymptotically a momentum $\mathbf{p}$. With the state ψ_f given by Eq. (2) we obtain $\hat{W} = \hat{W}_{1a} + \hat{W}_{2a} + \hat{W}_{12}$, where $\hat{W}_{ja}$ $(j = 1, 2)$ is the interaction between the jth electron and the nucleus of the atom and $\hat{W}_{12}$ is the electron-electron interaction.

In the correlated transfer ionization occurring in fast collisions ($v \gg Z_a$) both electrons undergo transitions in which the change of their momenta is much larger than their typical momenta in the initial atomic state. Because of that the nucleus of the atom is merely a spectator during this process [16]. Therefore, in order to find a suitable approximation for $\Psi_i^{(+)}(t)$ one can use the so-called impulse approximation, in which the role of the atomic nucleus is just to produce the momentum distribution (and binding energy) of the electrons in the initial state. Within this approximation we obtain

$$\Psi_i(t) = \frac{\exp[-i(v_a^2 + \epsilon_a)t]}{(2\pi)^3} \int d^3\boldsymbol{\kappa}_1 \int d^3\boldsymbol{\kappa}_2 \phi_a(\boldsymbol{\kappa}_1, \boldsymbol{\kappa}_2) \times \exp[-i(\boldsymbol{\kappa}_1 + \boldsymbol{\kappa}_2) \cdot \mathbf{R}_a(t)] \chi_{\mathbf{p}_1}^{(+)}(\mathbf{r}_1) \chi_{\mathbf{p}_2}^{(+)}(\mathbf{r}_2). \quad (3)$$

Here ϕ_a is the Fourier transform of the initial atomic state, $\mathbf{R}_a(t) = \mathbf{b} + \mathbf{v}_a t$ is a classical trajectory of the atomic nucleus moving with a velocity $\mathbf{v}_a$, and $-\epsilon_a$ is the atomic binding energy. Further, $\mathbf{p}_1 = \mathbf{v}_a + \boldsymbol{\kappa}_1$ and $\mathbf{p}_2 = \mathbf{v}_a + \boldsymbol{\kappa}_2$ are the initial momenta of the electrons with respect to the HCI and $\chi_{\mathbf{p}_j}^{(+)}(\mathbf{r}_j)$ $(j = 1, 2)$ are Coulomb wave functions of electrons which move in the field of the HCI having asymptotic momenta $\mathbf{p}_j$.

Using Eqs. (1)–(3) and assuming that the space part of the initial atomic state is symmetric under $\mathbf{r}_1 \overleftrightarrow{} \mathbf{r}_2$ one can show that in the projectile frame the cross section for the transfer ionization differential in the momentum $\mathbf{p}$ of the emitted electron is given by

$$\frac{d\sigma}{d^3\mathbf{p}} = \frac{1}{16\pi^2 v^2} \times \int d^2\mathbf{q}_\perp \left| \int d^3\boldsymbol{\kappa} \phi_a\left(\frac{\mathbf{q} + \boldsymbol{\kappa}}{2}, \frac{\mathbf{q} - \boldsymbol{\kappa}}{2} \right) W_{\mathrm{fi}} \right|^2. \quad (4)$$

Here,

$$\mathbf{q} = \left(\mathbf{q}_\perp, \frac{\varepsilon_f + p^2/2 - v_a^2 - \epsilon_i}{v_a} \right) \quad (5)$$

is the momentum transfer in the collision with $\mathbf{q}_\perp$ being its transverse part ($\mathbf{q}_\perp \cdot \mathbf{v}_a = 0$) and

$$W_{\mathrm{fi}} = \left\langle \chi_b(\mathbf{r}_1) \chi_{\mathbf{p}}^{(-)}(\mathbf{r}_2) \left| \frac{1}{r_{12}} \right| \chi_{\mathbf{p}_1}^{(+)}(\mathbf{r}_1) \chi_{\mathbf{p}_2}^{(+)}(\mathbf{r}_2) \right\rangle, \quad (6)$$

where $\mathbf{p}_1 = \mathbf{v}_a + (\mathbf{q} + \boldsymbol{\kappa})/2$ and $\mathbf{p}_2 = \mathbf{v}_a + (\mathbf{q} - \boldsymbol{\kappa})/2$.

Equation (4) can be simplified by noting that the Fourier transform $\phi_a((\mathbf{q} + \boldsymbol{\kappa})/2, (\mathbf{q} - \boldsymbol{\kappa})/2)$ becomes very small when $|\mathbf{q} \pm \boldsymbol{\kappa}|$ substantially exceed the typical electron velocities $\approx Z_a$ inside the atom. Since we assume that $v_a \gg Z_a$, we may set $\mathbf{p}_1 = \mathbf{p}_2 = \mathbf{v}_a$ and take $|W_{\mathrm{fi}}|^2$ in Eq. (4) out of the integrals.

Uncorrelated transfer ionization.—Let us now say a few words about the treatment of the uncorrelated transfer ionization. Following [8,14,16] we construct the amplitude for the ITI as the product of single-electron transition amplitudes for capture and ionization obtained using three-body models: continuum-distorted wave (for capture) and continuum-distorted-wave-eikonal-initial state (for ionization) [4].

Since the HCI's charge is large the C-SO, compared to the ITI, contributes negligibly. The emission produced by these channels is localized in the same part of the momentum space and the C-SO can simply be neglected.

Results and discussion.—In Figs. 1 and 2 we present results [21] for the momentum spectrum of electrons

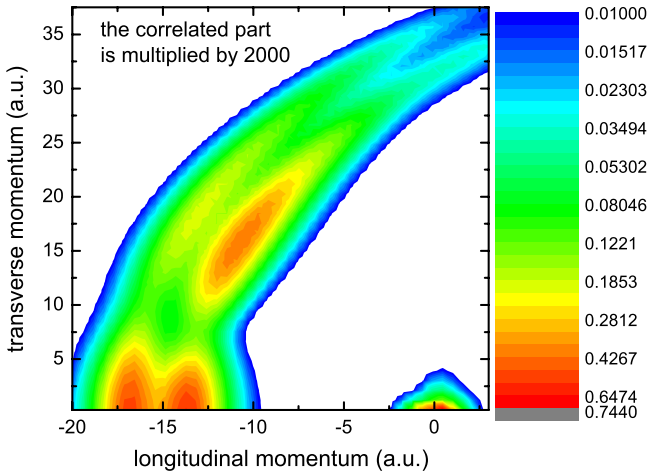

FIG. 1 (color online). Momentum spectrum [in b/(a.u.)3] of electrons emitted in the reactions 22.5 MeV/u $Ca^{20+} + He(1s^2) \rightarrow \sum_{n=1}^{2} Ca^{19+}(n) + He^{2+} + e^-$ ($v = 30$ a.u.). The contribution of the correlated channels is multiplied by 2000.

emitted in transfer ionization in collisions of 22.5 MeV/u Ca^{20+} ($v = 30$ a.u.) with helium atoms when capture occurs into the K and L shells. The spectrum is given in the target frame (= the laboratory frame) in which the HCI moves with a velocity $\mathbf{v}$ and is represented by the doubly differential cross section

$$\frac{d^2\sigma}{k_{\rm tr} dk_{\rm lg} dk_{\rm tr}} = \int_0^{2\pi} d\varphi_k \int d^2\mathbf{q}_\perp |S_{\rm fi}(\mathbf{q}_\perp)|^2, \qquad (7)$$

where $k_{\rm lg} = \mathbf{k} \cdot \mathbf{v}/v$ and $\mathbf{k}_{\rm tr} = \mathbf{k} - k_{\rm lg}\mathbf{v}/v$ are the longitudinal and transverse parts, respectively, of the momentum $\mathbf{k}$ of the emitted electron in the laboratory frame and $k_{\rm tr} = |\mathbf{k}_{\rm tr}|$. The integration in (7) runs over the transverse part of the momentum transfer and the azimuthal angle φ_k of the emitted electron.

In Fig. 1 the maximum at small momenta $k = |\mathbf{k}|$ has its origin in the ITI whereas the maxima at much larger k appear due to the correlated channels. The maximum at small k is very intense yielding a contribution of more than 90% to the total cross section. However, its structure is similar to that in fast collisions with low charged projectiles (see [16]) and will not be considered below.

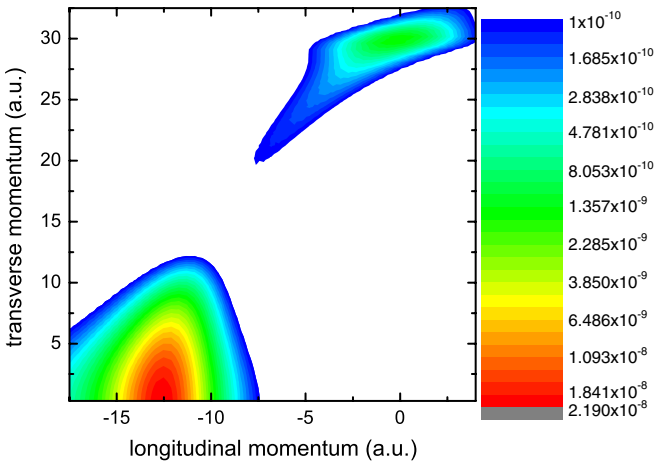

FIG. 2 (color online). Momentum spectrum [in b/(a.u.)3] of electrons emitted via the correlated mechanisms in the reaction 22.5 MeV $p^+ + He(1s^2) \rightarrow H(1s) + He^{2+} + e^-$.

Concerning the correlated transfer-ionization note that in the rest frame of the HCI, its (approximate) energy balance is given by $v^2 + \epsilon_a \approx -Z_i^2/2n^2 + p^2/2$, where n is the principal quantum number of the final bound state. Since $\mathbf{k}_{\rm tr} = \mathbf{p}_{\rm tr}$ and $k_{\rm lg} = v - p_{\rm lg}$, where $\mathbf{p}_{\rm tr}$ and $p_{\rm lg}$ are the transverse and longitudinal parts of $\mathbf{p}$, in the target frame the correlated emission is concentrated on ridges located along rings with radii $R_n = \sqrt{2v^2 + 2\epsilon_a + Z_i^2/n^2}$ centered at ($k_{\rm lg} = v$, $k_{\rm tr} = 0$).

The outer ridge in Fig. 1 arises due to the transfer ionization with electron capture into the ground state of the HCI while the inner ridge originates from capture into the L shell. Each of them has two distinct maxima centered at ($k_{\rm lg} \approx -16.8$, $k_{\rm tr} = 0$) and ($k_{\rm lg} \approx -12.8$, $k_{\rm tr} \approx 18.7$) for the outer ridge and at ($k_{\rm lg} \approx -13.6$, $k_{\rm tr} = 0$) and ($k_{\rm lg} \approx -10.6$, $k_{\rm tr} \approx 16$) for the inner one.

The shape of the correlated part of the spectrum in the case of collisions with HCIs is to be compared with that in collisions with low charged ions. The latter is displayed in Fig. 2 for 22.5 MeV $p^+ + He(1s^2)$ collisions. Since at $Z_i \ll v$ transfer ionization is strongly dominated by capture into the ground state, this spectrum [22] is concentrated on a single ridge. It consists of two distinct parts: the maximum centered at ($k_{\rm lg} \approx -12.5$, $k_{\rm tr} = 0$) is caused by the EEA mechanism whereas the maximum at ($k_{\rm lg} \approx 0$, $k_{\rm tr} \approx 30$) is due to the EET mechanism. Note that the ridge in Fig. 2 is shifted to lower k because of much smaller binding energy of the captured electron that results in smaller recoil for the other electron.

Comparing the spectra in Figs. 1 and 2, one can attribute the maxima at large negative $k_{\rm lg}$ and $k_{\rm tr} = 0$ in Fig. 1 to the EEA mechanism. However, in the strong-field regime there is no maximum at $k_{\rm lg} \approx 0$. Instead, a new maximum appears on each ridge which is absent for low charged ions. The contribution of this maximum to the total cross section is comparable to that of the EEA maximum.

Note that the new maximum may already appear when the HCI has a relatively low charge ($1 \ll Z_i \ll v$) but in such a case it has low intensity (see Fig. 3).

In order to get more ideas about the correlated transfer ionization in the strong-field regime, in Fig. 4 we present results for an even stronger field when 22.5 MeV/u Zn^{30+} collide with helium. From Fig. 4(a) one can see that the structure of the spectrum is similar to that in collisions with Ca^{20+} ions: it has two ridges and each of them has two pronounced maxima. Now, however, the maxima at large $k_{\rm tr}$ become noticeably more populated compared to those at $k_{\rm tr} \approx 0$.

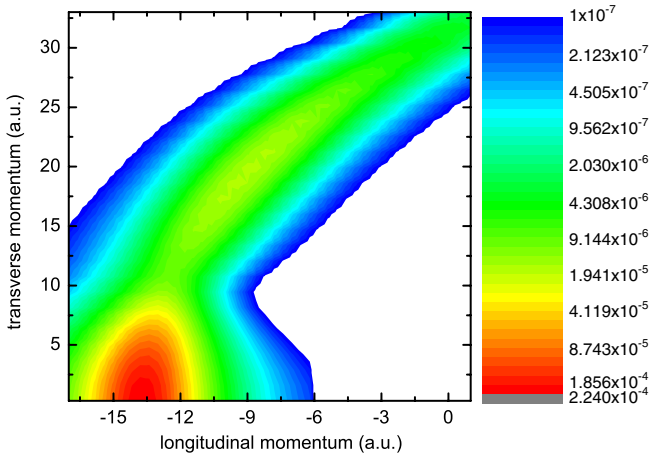

FIG. 3 (color online). Same as in Fig. 2 but for the reaction 22.5 MeV/u $Ne^{10+} + He(1s^2) \rightarrow Ne^{9} + (1s) + He^{2+} + e^{-}$.

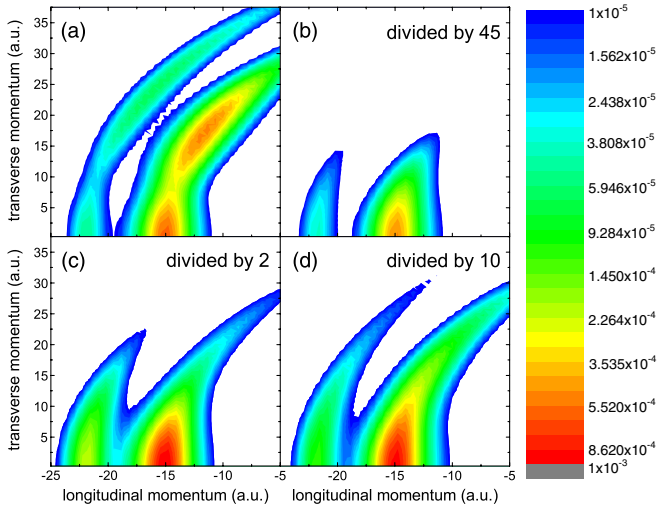

FIG. 4 (color online). The momentum spectra for the reactions 22.5 MeV/u $Zn^{30+} + He(1s^2) \rightarrow \sum_{n=1}^{2} Zn^{29+}(n) + He^{2+} + e^{-}$. The results in (b), (c) and (d) are divided by 45, 2, and 10, respectively.

Figure 4 also shows three more results. The spectrum presented in Fig. 4(b) was obtained by approximating all the states $\chi^{(+)}_{\mathbf{v}_a}(\mathbf{r}_1)$, $\chi^{(+)}_{\mathbf{v}_a}(\mathbf{r}_2)$ and $\chi^{(-)}_{\mathbf{p}}(\mathbf{r}_2)$ by plane waves. Figure 4(c) displays results calculated when $\chi^{(+)}_{\mathbf{v}_a}(\mathbf{r}_2)$ and $\chi^{(-)}_{\mathbf{p}}(\mathbf{r}_2)$ are modeled by plane waves whereas $\chi^{(+)}_{\mathbf{v}_a}(\mathbf{r}_1)$ is the Coulomb one. Finally, Fig. 4(d) shows the spectrum obtained if $\chi^{(+)}_{\mathbf{v}_a}(\mathbf{r}_1)$ is taken as a plane wave but $\chi^{(+)}_{\mathbf{v}_a}(\mathbf{r}_2)$ and $\chi^{(-)}_{\mathbf{p}}(\mathbf{r}_2)$ are Coulomb waves.

When the action of the HCI's field is neglected for both electrons (of course, except in the state χ_b) the spectrum has very pronounced EEA maxima and their intensity rapidly decrease when the transverse component k_{tr} of the electron momentum increases [see Fig. 4(b)].

If the field of the HCI is neglected only for that electron, which is finally emitted, the EEA maxima become less pronounced, the spectrum has more extension in the direction of larger k_{tr} but new maxima do not yet appear [see Fig. 4(c)]. If we neglect the action of the HCI's field on that electron which is finally captured, but take into account HCI's action on the other electron, the spectrum extends even more in the transverse direction, but new maxima are still absent [see Fig. 4(d)].

And only when the action of the HCI's field on the electrons is fully included, do new maxima appear [Fig. 4(a)]. In this case the EEA maxima further decrease in intensity and the extension of the spectrum in the direction of large k_{tr} is most pronounced.

Thus, the action of the HCI's field on *both* electrons in the continuum is necessary for the second maxima to appear. Therefore, they are a signature of a new reaction mechanism qualitatively different from the EET mechanism which proceeds via the interaction between the incident ion and only *one* of the atomic electrons.

In conclusion, we have considered transfer ionization in collisions of helium with fast nuclei having so high of a charge Z_i that $Z_i \sim v \gg Z_a$. We focused on the correlated channels of this process in which the electron-electron interaction during the collision plays a crucial role. Our results were obtained using a treatment which enables one to fully account for the action of the strong field generated by a highly charged ion on the electrons.

Our consideration shows that the strong field has a profound effect on the correlated transfer ionization. Compared to the weak-field regime realized in collisions with low charged ions, the strong field weakens (in relative terms) the EEA mechanism and eliminates the EET mechanism. Instead, a new reaction mechanism appears whose intensity increases with the field strength.

The correlated transfer ionization is intimately related to the process of radiative two-electron transfer in which two atomic electrons are captured by the projectile with emission of a single photon. Indeed, the electron ejected in transfer ionization can recombine radiatively with the projectile leading to the radiative two-electron transfer. Since the probability of radiative recombination is very low, this process has much smaller cross sections than the transfer ionization that makes it very difficult for experimental observation [23]. Therefore, further studies of transfer ionization [24] may also shed more light on the correlated two-electron–one-photon capture.

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[24] According to discussions with D. Fischer and P. Mokler, an experimental test of our predictions is feasible.