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Shakeover probability for electron capture

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The simple shake probability for electron capture is formulated and evaluated for 1*s*-1*s* electron capture at high collision velocity v for projectiles and targets of charge Z_P and Z_T, respectively. By introducing orthogonalized wave functions, corresponding to asymptotically correct first Born calculations, a shake probability is obtained that goes to zero when the electron screening s remains unchanged during the collision. When $Z_T \neq Z_P$, our shake probability varies as $Z_< Z_>^5 s^2/v^8$, where $Z_{<(>)}$ is the smaller (larger) of Z_P and Z_T. First Born probabilities vary as $Z_P^5 Z_T^5/v^{12}$. A minimum in the shake probability is predicted for charge-symmetric systems.

I. INTRODUCTION

Multiple electron transitions in atomic collisions can sometimes give more direct insight into many-body effects than transitions of a single electron where many-body effects are often of secondary importance. Recent studies[1–5] of double ionization in helium by protons and antiprotons, for example, have led to new understanding of the interplay of independent-electron and shakeoff mechanisms for double ionization. For electron capture some studies exist using the independent-electron approximation,[6–9] but no proper theory for a shake process in electron capture has yet been developed.[8] In this paper we formulate and evaluate simple shake amplitudes and probabilities for electron capture. This shake process, called shakeover, occurs when a second electron is captured due to a change in nuclear screening accompanying capture of a first electron by the projectile.

The shake concept has been used in multiple ionization for many years.[10–13] In the simple shake picture, the probability for ionization of a second electron is $|\langle \phi_f | \phi_i \rangle|^2$. If there is a change in screening then the unperturbed final-state Hamiltonian H_{0f} differs from the initial state H_{0i} and ϕ_i a superposition of final eigenstates, i.e., $\phi_i = \sum_f a_{if}\phi_f$. When there is no change in screening then $\langle \phi_f | \phi_i \rangle$ is zero for $f \neq i$. In other words, there is a physical cause for the nonorthogonality of ϕ_i and ϕ_f, namely, a change in screening. This point requires special attention in the case of electron capture. In this simple shake picture the ratio of single to double ionization cross sections, $R = |\langle \phi_f | \phi_i \rangle|^2$, is independent of the projectile charge and velocity. For electron capture the electron is translating in the final state so that $\langle \phi_f | \phi_i \rangle$ becomes velocity dependent.

Understanding of double capture rests to a large degree upon the understanding of single capture. For total cross sections for single capture most properties, such as the charge and to some extent the velocity dependence, can be understood in terms of simple first Born cross sections. Quantitative agreement with most observations at high velocity has been obtained by using a first Born approximation which is asymptotically correct.[14–20] This approximation may be obtained from the simple Brinkman-Kramer version of the first Born approximations by a Gramm-Schmidt orthogonalization of the final state with respect to the initial state.[21] In this paper we shall use these first Born approaches as a standard of comparison for total cross sections, ignoring for the most part second Born effects which can be important in differential cross sections and which, at very high energies, modify slightly the velocity dependence of the total cross section.

Most existing calculations[6–9] of double-electron capture are based on the independent-electron approximation in which the probability for capturing two electrons (e.g., from helium) is $P_1 P_2$ when P_i is the probability of capturing the ith electron ($i = 1,2$). Recently, Miraglia and Gravielle[8] have pointed out that at high velocities the independent-electron approximations may not give the dominant contribution to double-electron capture and that proper treatment of the orthogonality properties of ϕ_i and ϕ_f is important in understanding double capture at high velocities.

In this paper we formulate and evaluate the shakeover probability for electron capture. Our formulation includes orthogonalization so that the shakeover probability goes to zero as the change in screening goes to zero. We also consider in screening in both the target and the projectile. We discuss some of the limitations of one simple shake probability, and consider extension to a generalized shake probability including electron exchange and initial-state correlation. Here we use atomic units where $e^2 = \hbar = m_e = 1$.

II. FORMULATION

In the impact-parameter representation[22] the exact probability amplitude for a transition from ϕ_i to ϕ_f is

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given[5] to first order in the electron-projectile interaction V by

$$a_{if}(\mathbf{B})=\langle \phi_f \mid \psi_i \rangle = \langle \phi_f \mid U_I(+\infty,-\infty) \mid \phi_i \rangle = \left\langle \phi_f \left| T \exp\left[-i \int_{-\infty}^{\infty} V_I(t)dt \right] \right| \phi_i \right\rangle = \left\langle \phi_f \left| 1 - i \int_{-\infty}^{\infty} V_I(t)dt \right| \phi_i \right\rangle . \quad (1)$$

Here V_I and the evolution operator U_I are expressed in the interaction representation where it is assumed that the projectile trajectory $\mathbf{R}(t)$ is known, i.e., $\mathbf{R}=\mathbf{B}+\mathbf{v}t$, and that no transition occurs if there is no interaction with the projectile so that the first term at the end of Eq. (1) is zero.

We now consider the simple shake probability for a two-electron system. For the simple shake probability both correlation and antisymmetrization of the electron wave functions are ignored, so that $\phi=\phi(\mathbf{r}_1)\phi(\mathbf{r}_2)$. For uncorrelated wave functions the asymptotic Hamiltonian is a sum of single-particle terms, e.g., $H_0=-\frac{1}{2}\nabla_1^2 - Z_T/r_1 - \frac{1}{2}\nabla_2^2 - Z_T/r_2$. For shakeoff to occur H_{0i} and H_{0f} must differ. In this paper the nuclear charge Z_T is set equal to $Z_T - s$ in the initial state and Z_T in the final state. Consequently, ϕ_f and ϕ_i are nonorthogonal unless the change in searching screening s is zero. There is a similar contribution from the change in screening of the projectile as $Z_P \to Z_P - s$, except that the screening increases in Z_P and decreases in Z_T.

Now $V_I = V_I^1 + V_I^2$ in Eq. (1) and noting that V_I^1 acts only on $\phi(\mathbf{r}_1)$ and V_I^2 on $\phi(\mathbf{r}_2)$, we have

$$a_{if} = -i\left\langle \phi_f(\mathbf{r}_1)\phi_f(\mathbf{r}_2) \left| \int_{-\infty}^{\infty} V_I^1 dt + \int_{-\infty}^{\infty} V_I^2 dt \right| \phi_i(\mathbf{r}_1)\phi_i(\mathbf{r}_2) \right\rangle = -i\left[\int_{-\infty}^{\infty} \langle \phi_f(\mathbf{r}_1) \mid V_I^1 \mid \phi_i(\mathbf{r}_1)\rangle dt \langle \phi_f(\mathbf{r}_2) \mid \phi_i(\mathbf{r}_2)\rangle + \int_{-\infty}^{\infty} \langle \phi_f(\mathbf{r}_2) \mid V_I^2 \mid \phi_i(\mathbf{r}_2)\rangle dt \langle \phi_f(\mathbf{r}_1) \mid \phi_i(\mathbf{r}_1)\rangle \right] . \quad (2)$$

In this amplitude one electron is captured and the other undergoes a shake transition, corresponding to $\langle \phi_f \mid \phi_i \rangle \neq 0$.

Let us consider double capture and specify that electron 1 is captured and electron 2 is the shake electron. Now ϕ_i and ϕ_f are most conveniently expressed in terms of $\mathbf{r}_T$ and $\mathbf{r}_P$ where $\mathbf{r}_{T(P)}$ is the position of the electron relative to the target (projectile) nucleus. Then

$$a_{if} = -i\int_{-\infty}^{\infty} \langle \phi_f^*(\mathbf{r}_{1P}) \frac{Z_P}{\mid \mathbf{B}+\mathbf{v}t-\mathbf{r}_{1T} \mid} \phi_i(\mathbf{r}_{1T}) \rangle dt \times \langle \phi_f(\mathbf{r}_{2P}) \mid \phi_i(\mathbf{r}_{2T}) \rangle = a_{\text{cap}} \langle \phi_f(\mathbf{r}_{2P}) \mid \phi_i(\mathbf{r}_{2T}) \rangle = a_{\text{cap}} S . \quad (3)$$

The simple amplitude for double capture factors into a capture amplitude and a shakeover amplitude S. Consequently, a_{if} is uncorrelated. In particular, the time integration originating in Eq. (1) does not extend[23] over the shake amplitude in the impact-parameter picture. We specify $\mathbf{r}_{2P}=\mathbf{R}+\mathbf{r}_{2T}$ by specifying that $Z_T - s$ changes to Z_T and Z_P to $Z_P - s'$ at $t=0$.

Next let us address the question of orthogonality. To avoid spurious effects[14–16] due to nonorthogonality we use a Gramm-Schmidt procedure[21] to orthogonalize ϕ_f to ϕ_i when $s=s'=0$. We note that this procedure gives a first Born amplitude that corresponds to the asymptotically correct amplitude[14–20] and gives better agreement with experiment than the simpler "nonorthogonal" Brinkman-Kramer amplitude. Specifically we use

$$\phi'_{f\perp}(Z_T,Z_P-s') = \phi'_f(Z_T,Z_P-s') - \langle \phi'_f(Z_T,Z_P-s') \mid \phi'_i(Z_T,Z_P-s') \rangle \phi'_i(Z_T,Z_P-s')$$

or

$$\phi'_{f_\perp} = \phi'_f - \langle \phi'_f \mid \phi'_i \rangle \phi'_i . \quad (4)$$

This means that the final state ϕ'_f where $s=0$ $s'\neq 0$ is orthogonal to a ground state ϕ'_i, where $s=0$ and $s'\neq 0$. The initial state ϕ_i corresponds to $Z_T - s$, and Z_P, i.e., $s\neq 0$ and $s'=0$, the reverse of ϕ'_f and ϕ'_i.

Now, the simple shakeover probability P_S may be expressed from Eqs. (3) and (4) by

$$P_S = \mid \langle \phi'_{f_\perp} \mid \phi_i \rangle \mid^2 = \mid \langle \phi'_f \mid \phi_i \rangle - \langle \phi'_f \mid \phi'_i \rangle \langle \phi'_i \mid \phi_i \rangle \mid^2 = \mid S_\perp \mid^2 = \mid S - S' \langle \phi'_i \mid \phi_i \rangle \mid^2 . \quad (5)$$

Here $\phi'=\phi(Z_T,Z_P-s')$ and $\phi=\phi(Z_T-s,Z_P)$ and S' is an overlap of ϕ'_i and ϕ'_f. As s and s' both go to zero, both $S_\perp$ and P_S reduce to zero. We note that s and s' are not strongly dependent on Z. In a variational calculation[24] $s=s'=\frac{5}{16}$, independent of Z to first order in an expansion in $1/Z$ for $1s$ electrons.

III. EVALUATION

The evaluation of the shakeover probability of Eq. (5) above is done by evaluating the overlap $\langle \phi'_{f_\perp} \mid \phi_i \rangle$ for arbitrary Z_P and Z_T. First we vary the screening s in Z_T and find the contribution which goes to zero as s goes to zero. Then we do the same for a change in screening s' of Z_P and combine both effects.

A. Overlap integral $\mathcal{S}$

Following a standard technique,[25] we consider for unscreened Z_T and Z_P,

$$\mathcal{S}=\langle \phi_f'(\mathbf{r}_P)\,|\,\phi_i'(\mathbf{r}_T)\rangle =\int e^{-i\mathbf{v}\cdot\mathbf{r}}\phi_f^*(\mathbf{r}-\tfrac{1}{2}\mathbf{R})\phi_i(\mathbf{r}+\tfrac{1}{2}\mathbf{R})d\mathbf{r} \tag{6}$$

at $\mathbf{R}=\mathbf{B}$ where $e^{-i\mathbf{v}\cdot\mathbf{r}}$ is the translation factor for electron capture. For $1s$-$1s$ capture using

$$\tilde{\phi}(\mathbf{p})=(2\pi)^{3/2}\int \phi(\mathbf{r})e^{i\mathbf{p}\cdot\mathbf{r}}d\mathbf{r}=\sqrt{8}Z^{5/2}/\pi(p^2+Z^2)^2 ,$$

one has

$$\begin{aligned}\mathcal{S}&=\frac{1}{(2\pi)^3}\int d\mathbf{k}\int d\mathbf{K}\,\tilde{\phi}_f^*(\mathbf{k})\tilde{\phi}_i(\mathbf{K})e^{-(1/2)i\mathbf{R}\cdot(\mathbf{k}+\mathbf{K})}\\&\quad\times\int d\mathbf{r}\,e^{-i\mathbf{r}\cdot(\mathbf{K}-\mathbf{k}+\mathbf{v})}\\&=e^{-(1/2)i\mathbf{R}\cdot\mathbf{v}}\int d\mathbf{K}\,\phi_f(\mathbf{K}+\mathbf{v})\phi_i(\mathbf{K})e^{-i\mathbf{K}\cdot\mathbf{B}}\\&=\frac{8}{\pi^2}(Z_PZ_T)^{5/2}\int d\mathbf{K}\frac{e^{-i\mathbf{K}\cdot\mathbf{B}}}{[Z_P^2+(\mathbf{K}+\mathbf{v})^2]^2(Z_T^2+K^2)^2} ,\end{aligned} \tag{7}$$

where $\mathbf{R}=\mathbf{B}$ and $\mathbf{B}\cdot\mathbf{v}=0$.

Using a peaking approximation to first order in v/Z and standard integrals,[26] we have

$$\begin{aligned}\mathcal{S}&\cong\frac{8}{\pi^2v^4}(Z_PZ_T)^{5/2}\int d\mathbf{K}\,e^{i\mathbf{K}\cdot\mathbf{B}}\left[\frac{1}{[Z_P^2+(\mathbf{K}+\mathbf{v})^2]^2}+\frac{1}{(Z_T^2+K^2)^2}\right]\\&=\frac{8}{\pi^2v^4}(Z_PZ_T)^{5/2}2\pi\int_0^\infty K^2dK\left[\frac{1}{(Z_P^2+K^2)^2}+\frac{1}{(Z_T^2+K^2)^2}\right]\int_{-1}^{1}e^{iKB\cos\phi}d(\cos\phi)\\&=\frac{8}{\pi v^4}(Z_PZ_T)^{5/2}\left[\frac{4\pi}{B}\lim_{\lambda\to Z_P}\left[\frac{-1}{2\lambda}\frac{d}{d\lambda}\right]+\frac{4\pi}{B}\lim_{\lambda\to Z_T}\left[\frac{-1}{2\lambda}\frac{d}{d\lambda}\right]\right]\int_0^\infty\frac{K\sin KB}{\lambda^2+K^2}dK\\&=\frac{8(Z_PZ_T)^{5/2}}{v^4}\left[\frac{e^{-Z_PB}}{Z_P}+\frac{e^{-Z_TB}}{Z_T}\right] .\end{aligned} \tag{8}$$

For screened Z_T one simply replaces Z_T by Z_T-s. Screening in Z_P is treated similarly.

B. Shake overlap $S-S'$ at $s'=0$

Here we evaluate $S'-S$ for no change in Z_P, i.e., $s'=0$. In Sec. III D we add the contribution for $Z_P\to Z_P-s'$. This enables us to consider the effect of target and projectile screening separately. Finding $S-S'$ at fixed s' is simply done by subtracting Eq. (8) with $Z_T\to Z_T-s$ from Eq. (8) with Z_T. Setting $Z_T-s\equiv Z_T(1-\epsilon)$ we have, expanding to first order in $\epsilon=s/Z_T$,

$$\begin{aligned}S-S'_{s'=0}&=\frac{8}{v^4}[Z_PZ_T(1-\epsilon)]^{5/2}\left[\frac{e^{-Z_PB}}{Z_P}+\frac{e^{-Z_T(1-\epsilon)B}}{Z_T(1-\epsilon)}\right]-\frac{8(Z_PZ_T)^{5/2}}{v^4}\left[\frac{e^{-Z_PB}}{Z_P}+\frac{e^{-Z_TB}}{Z_T}\right]\\&=\frac{-8(Z_PZ_T)^{5/2}}{v^4}\left[\frac{s}{Z_T}\right]\left[\frac{5}{2}\frac{e^{-Z_PB}}{Z_P}+(\tfrac{3}{2}-Z_TB)\frac{e^{-Z_TB}}{Z_T}\right]+O\left[\frac{s^2}{Z_T^2}\right] .\end{aligned} \tag{9}$$

Here Z_P does not change.

C. Ground-state overlap $\langle\phi_i'\,|\,\phi_i\rangle$

For $1s$ hydrogenic ground-state wave functions we have, again using $\epsilon=s/Z_T$,

$$\begin{aligned}\langle\phi_i'\,|\,\phi_i\rangle&=\int d\mathbf{r}\phi_i^*(Z_T)\phi_i(Z_T-s)\\&=[Z_TZ_T(1-\epsilon)]^{3/2}\int_0^\infty e^{-(Z_T+Z_T-s)}r^2dr\\&=\frac{[Z_T^2(1-\epsilon)]^{3/2}}{[Z_T(1-\epsilon/2)]^3}\cong 1-\frac{3}{8}\frac{s^2}{Z_T^2}+O\left[\frac{s^3}{Z_T^3}\right] .\end{aligned} \tag{10}$$

Since the correction from s is of order $\epsilon^2=s^2/Z_T^2$ it may be ignored to first order in s/Z_T. A similar result holds for $Z_P\to Z_P-s'$.

D. Amplitude with changes in both Z_T and Z_P

The shakeover amplitude for $Z_T-s\to Z_T$ and $Z_P\to Z_P-s'$ may be found subtracting from Eq. (9) a similar amplitude with Z_T replaced by Z_P and s by s'. The amplitudes are subtracted because the screening increases for Z_P and decreases for Z_T during the collision. The result is readily found to be

$$(S-S')=\frac{8}{v^4}(Z_PZ_T)^{5/2}\times\left[\left[(\tfrac{3}{2}-Z_PB)\frac{s'}{Z_P}-\frac{5}{2}\frac{S}{Z_T}\right]\frac{e^{-Z_PB}}{Z_P}+\left[\frac{5}{2}\frac{s'}{Z_P}-(\tfrac{3}{2}-Z_TB)\frac{s}{Z_T}\right]\frac{e^{-Z_TB}}{Z_T}\right]. \tag{11}$$

This is the shakeover amplitude to first order in s/Z_P and s'/Z_P.

E. Shakeover probability P_S

The shakeover probability P_S, for 1*s*-1*s* capture is now readily found from Eqs. (5), (10), and (11), namely,

$$\begin{aligned}P_S(B)&=|S_\perp|^2=|S-S'\langle\phi_i'|\phi_i\rangle|^2\\&\simeq|S-S'|^2\\&=\frac{64}{v^8}Z_P^5Z_T^5\left[\left[(\tfrac{3}{2}-Z_PB)\frac{s'}{Z_P}-\frac{5}{2}\frac{s}{Z_T}\right]\frac{e^{-Z_PB}}{Z_P}+\left[\frac{5}{2}\frac{s'}{Z_P}-(\tfrac{3}{2}-Z_TB)\frac{s}{Z_T}\right]\frac{e^{-Z_TB}}{Z_T}\right]^2.\end{aligned} \tag{12}$$

This corresponds to Z_T-s changing to Z_T and Z_P changing to Z_P-s' at $t=0$. It is useful to note that at $B=0$ one has

$$P_S(0)=\frac{16}{v^8}Z_P^5Z_T^5\left[3\left[\frac{s'}{Z_P^2}-\frac{s}{Z_T^2}\right]+\frac{5}{Z_PZ_T}(s'-s)\right]^2. \tag{13}$$

$P_S(B)$ goes to zero as both s and s' go to zero.

IV. RESULTS AND DISCUSSION

The simple shakeover probability, unlike simple shakeoff and shakeup, is dependent on the parameters describing the projectile. That is, P_S in Eq. (11) varies with v, Z_P, and B, as well as the target parameters Z_T and s. The v^{-8} dependence comes from the $e^{i\mathbf{v}\cdot\mathbf{r}}$ translation factor in Eq. (6), and the Z_P and B dependence also arises because the electron leaves in the ground state of the projectile. The effect due to the change in screening s is linear in the shakeover amplitude and quadratic in the probability. This corresponds to a first-order perturbation effect in s. In this regard, shakeover, shakeoff, and shakeup are similar, namely, the shake effect in the probability varies as s^2/Z_T^2 to first order.

At sufficiently high velocities shakeover will dominate over direct double capture. For simple estimates, we compare our simple shakeover probability to the Brinkman-Kramer (BK) probability for direct 1*s*-1*s* electron capture given by

$$P_{\rm BK}(B)=\frac{4Z_P^5Z_T^5}{Z_T^8v^2}\frac{[X^2K_2(X)]^2}{(1+S^2/4)^4}\rightarrow\frac{2^{12}Z_P^5Z_T^5}{v^{10}},\quad \text{as } B\rightarrow 0\ ,$$

where

$$X=BZ_T(1+S^2/4)^{1/2}\ ,\qquad S=\frac{v}{Z_T}\left[1-\frac{(Z_T-Z_P)^2}{v^2}\right]. \tag{14}$$

Note that as v increases the mean impact parameter contributing to capture becomes small, i.e., $B \ll Z_T$ and Z_P. This suggests that to a good approximation we can take $B \ll Z_T$ in the shakeoff probability in Eq. (1). Then for double-capture cross sections due to the direct (or independent-electron approximation) and shakeover mechanism we have

$$\sigma_{\rm IEA}^{++}=2\pi\int_0^\infty P_{\rm cap}(B)P_{\rm cap}(B)B\,dB\ , \tag{15a}$$

$$\sigma_S^{++}=P_S(0)2\pi\int_0^\infty P_{\rm cap}(B)B\,dB=\frac{16}{v^8}Z_P^5Z_T^5\left[3\left[\frac{s'}{Z_P^2}-\frac{s}{Z_T^2}\right]+\frac{5}{Z_PZ_P}(s'-s)\right]^2\sigma^+\ , \tag{15b}$$

where σ^+ is the single-capture cross section. To first order in s/Z, our shakeover probability goes to zero when $s=s'$ and $Z_P=Z_T$, i.e., for charge-symmetric systems.

A very rough estimate of the velocity above which shakeover dominates direct double capture is found by noting that the BK cross sections and probabilities are often an order of magnitude too large. Taking $s'=s$ and

$$1<\frac{P_S(0)}{\frac{1}{10}P_{\rm BK}(0)}=\frac{v^2 10(3s)^2}{2^8}\left[\frac{1}{Z_P^2}-\frac{1}{Z_T^2}\right]^2$$

or

$$v\gtrsim\frac{2^4}{10s}\left[\frac{1}{Z_P^2}-\frac{1}{Z_T^2}\right]^{-1}, \tag{16}$$

for $s=0.3$ and $Z_P\neq Z_T$, we have $v\gtrsim 5Z_<^2$. For $Z_<=2$ this corresponds to velocities above 10 MeV/amu. Since the numerical coefficient of the simple shake probability could easily be in error by a factor of 10, crossover velocity could be in error by a factor of 10 or more.

A comparison for double-capture cross sections and for the ratio of double- to single-electron capture, $R=\sigma^{++}/\sigma^+$, is given in Table I. The continuum-

TABLE I. Charge and velocity dependence of double-electron capture.

Model	σ^{++}	$R=\sigma^{++}/\sigma^{+}$
Independent-electron approximation (first Born)	$\frac{Z_P^{10}Z_T^{10}}{v^{22}}$	$\frac{Z_P^5Z_T^5}{v^{10}}$
Shakeover (first Born)	$\frac{Z_P^{10}Z_T^{10}s^2}{v^{20}}\left[\frac{1}{Z_P^2}-\frac{1}{Z_T^2}\right]^2$	$\frac{Z_P^5Z_T^5s^2}{v^8}\left[\frac{1}{Z_P^2}-\frac{1}{Z_T^2}\right]^2$
CDW (TEM) [Gravielle and Miraglia Ref. 8(b)]	$\frac{Z_P^{10}Z_T^{10}}{v^{18}(Z_T+Z_P)^4}$	$\frac{Z_P^5Z_T^5}{v^7(Z_T+Z_P)^4}$

distorted wave (CDW) calculations of Gravielle and Miraglia,[8(b)] using peaking approximations, also include effects of the second-order Thomas peak which modify the v-dependence single-capture cross sections by one power of v at asmptotically high v. The various results in Table I differ in the Z_P, Z_T, and v dependences.

Experimental tests of double-electron capture at high velocity could provide a helpful guide in understanding this phenomenon. The cross sections are very small. For 10-MeV protons on helium a strong potential Born (SPB) calculation gives a single-capture cross section of about 10^{-26} cm^2, and using Eq. (13) we estimate a double-capture cross section of 5×10^{-35} cm^2. However, the development of storage rings[27] may make these experiments feasible. We point out that determination of the velocity and/or charge dependences of the ratio of double to single capture at high velocity would provide useful information.

Our shakeover probability can also be used to evaluate cross sections at high collision velocities for simultaneous capture and ionization of two electrons, i.e., transfer ionization. This gives a transfer ionization cross section which varies as $P_{\text{ion}}P_{\text{shake}}\sim v^{-2}v^{-8}=v^{-10}$. In this case the ratio of transfer ionization to single capture, $R=\sigma^{++}/\sigma^{+}$, varies as v^2 (or v^1 if we include the Thomas peak). Then the ratio R is predicted to increase slightly with increasing velocity and this mechanism eventually dominates over single capture plus shakeoff.

Our simple shakeover calculation has a number of limitations. The simple shakeover calculations do not include initial-state correlation or antisymmetrization of the electron wave functions, both of which should be included in generalized shakeoff probabilities.[13] Initial-state correlation significantly alter the numerical coefficient of our shakeover probability, and possibly the Z_P and Z_T dependence, but we do not expect the v dependence to change significantly. Final-state correlation and Coulombic distortions in the wave functions could affect the shake probability somewhat if the velocity is not too high. Second-order effects such as the singularity that gives rise to the Thomas peak could become important at energies above $100Z_T^2$ MeV/amu where the Thomas peak begins to influence the total single-capture cross section. However, we have found no reason to expect the simple shake probability of Eq. (11) to be affected. We do expect the shakeover result to be the same in the wave picture as in our impact-parameter picture first order in Z/v and s/Z. At energies above one may expect radiative electron capture (REC) to play a significant role, although we expect the analysis given here to apply to radiative as well as nonradiative electron capture.

For double-capture cross sections, which are quite small at high velocities, it is difficult to rule out the possibility of processes not yet considered. Perhaps there is four-body amplitude, possibly analogous to the Thomas singularity, which is larger than the small effects considered here. Experimental data, when it is possible to obtain, would be quite helpful in guiding our understanding of double-electron capture at high velocity.

V. SUMMARY

We have formulated and evaluated the simple shakeover probability for electron capture at high velocity. Shakeover of a second electron occurs when there is a change of screening in either the target or the projectile when a first electron is captured. Our simple shakeover probability for 1s-1s capture with Z_P and Z_S changing by $-s$ and $+s$, respectively, varies at small impact parameters as

$$\frac{Z_T^5Z_P^5s^2}{v^8}\left[\frac{1}{Z_P^2}-\frac{1}{Z_T^2}\right]^2$$

with a minimum at $Z_P=Z_T$.

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$$\begin{aligned} a_{\text{if}} &\cong \left\langle \phi_f \,\middle|\, \int V_1(t_1)dt_1 \int V_2(t_2)dt_2 \,\middle|\, \phi_i \right\rangle \\ &= \int dt_1 \langle \phi_f^1 | V_1 | \phi_i^1 \rangle \int dt_2 \langle \phi_f^2 | V_2 | \phi_i^2 \rangle \\ &= a_1 a_2 \ . \end{aligned}$$

This may be derived from Eq. (1) (cf. Ref. 5).

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