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Second Born approximation with the Coulomb Green's function: Electron capture from a hydrogenlike ion by a bare ion

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We have applied the second Born approximation with the *Coulomb* Green's function to the calculation of the cross section for electron capture from a hydrogenlike ion of high atomic number Z_T by a bare ion of atomic number Z_P moving with a high speed v. With the aid of a peaking approximation, which is valid when $\hbar v/e^2 \gg Z_P$ and $Z_T \gg Z_P$, we reduced the second Born amplitude to a one-dimensional integral which was evaluated numerically for $1s \rightarrow 1s$ capture. It was found that by using the Coulomb Green's function, rather than the *free* Green's function, the second Born cross section is greatly reduced (and is comparable in size to the first Born cross section) when $\hbar v/e^2 \lesssim Z_T$.

I. INTRODUCTION

Inner-shell electron capture by swiftly moving projectiles is a complicated theoretical problem owing in part to the presence of many electrons interacting with the active electron. To progress towards an understanding of the dynamics of inner-shell electron capture we have begun by studying the simpler process of electron capture from a hydrogenlike ion of high atomic number Z_T by a bare ion of atomic number Z_P moving with a high speed v. It is now well-known[1] that if $\hbar v/e^2 \gg Z_T, Z_P$, the second Born amplitude dominates over the first. (We omit the internuclear potential from each Born amplitude.) With v satisfying the previous inequalities it makes little difference whether the free Green's function or the Coulomb Green's function is used in the definition of the second Born amplitude. In a recent letter one of us[2] evaluated the second Born amplitude (for $1s \rightarrow 1s$ capture) with the *free* Green's function for $\hbar v/e^2 \gg Z_P$ and Z_T arbitrary. It was found that the ratio of the second and first Born cross sections increases rapidly with Z_T and is very large for $\hbar v/e^2 \lesssim Z_T$. (For example, if $Z_P = 1$ and $\hbar v/e^2 = Z_T = 10$ the ratio is nearly 15.) It is to be expected that the contribution from terms of third and higher order in the interaction between the electron and target nucleus is significant when $\hbar v/e^2 \lesssim Z_T$. Now all orders in this interaction can be incorporated in the Coulomb Green's function. We have therefore examined the second Born amplitude using the Coulomb Green's function, and the purpose of this paper is to report the results. We find that (for $1s \rightarrow 1s$ capture) the ratio of the second and first Born cross sections is greatly reduced if the Coulomb, rather than the free, Green's function is used when $\hbar v/e^2 \lesssim Z_T$. Hence when the free Green's function is used, the second Born amplitude must destructively interfere with higher-order Born amplitudes.

In the next section we establish a notation. In Sec. III we analyze the required matrix element of the Coulomb Green's function. This matrix element is evaluated using a peaking approximation which is valid when $\hbar v/e^2 \gg Z_P$ and $Z_T \gg Z_P$. In Sec. IV we present the results and a discussion of them. In the Appendix we show that the matrix element of the Coulomb Green's function with the peaking approximation reduces to the familiar matrix element of the free Green's function when $\hbar v/e^2 \gg Z_T \gg Z_P$.

II. NOTATION

Let M_P be the mass of a projectile P impinging on a one-electron ion or atom $(e+T)$, where e is the electron of mass m, and T is the target nucleus of mass M_T. We define the mass ratios

$$\alpha = M_T/(m+M_T), \quad \beta = M_P/(m+M_P),$$

and the reduced masses

$$\nu_i = M_P(m+M_T)/(m+M_T+M_P),$$

$$\nu_f = M_T(m+M_P)/(m+M_T+M_P).$$

Let $\vec{r}_T$ and $\vec{r}_P$ be the coordinates of the electron relative to T and to P, respectively. Let $\vec{R}_T$ be the coordinate of P relative to the center of mass of $(e+T)$ and let $\vec{R}_P$ be the coordinate of the center of mass of $(e+P)$ relative to T. Let $\vec{R}$ be the coordinate of P relative to T. The coordinate system is shown in Fig. 1. We have

$$\vec{r}_P = -\vec{R}_T + \alpha\vec{r}_T, \quad \vec{R}_P = \beta\vec{R}_T + (1-\alpha\beta)\vec{r}_T.$$

Let $-e$ denote the electron charge, and let $Z_T e$ and $Z_P e$ be the charges of T and P, respectively.

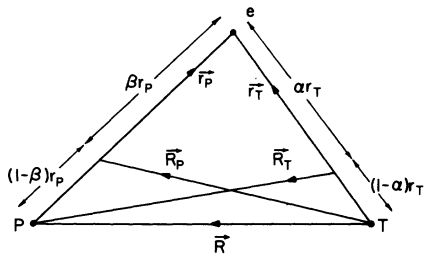

FIG. 1. The coordinate system.

Let ϵ_i be the internal energy of $(e+T)$ in the initial state i and let ϵ_f be the internal energy of $(e+P)$ in the final state f. Unless stated otherwise, we work in the center-of-mass frame of all three particles. In this frame the total energy E of the system is

$$E=(\hbar^2/2\nu_i)K_i^2+\epsilon_i=(\hbar^2/2\nu_f)K_f^2+\epsilon_f\,,$$

where $\hbar\vec{K}_i$ is the initial momentum of P, and $\hbar\vec{K}_f$ is the final momentum of $(e+P)$, with $K_i=|\vec{K}_i|$ and $K_f=|\vec{K}_f|$. With $\vec{v}$ the incident velocity of P relative to the center of mass of $(e+T)$, we have $\hbar\vec{K}_i=\nu_i\vec{v}$. We define the "average" momentum transfer vectors

$$\vec{K}=\beta\vec{K}_f-\vec{K}_i,\quad \vec{J}=\alpha\vec{K}_i-\vec{K}_f\,.$$

Let $\phi_i(\vec{r}_T)$ represent the initial internal state of $(e+T)$ and let $\phi_f(\vec{r}_P)$ represent the final internal state of $(e+P)$. The initial and final wave functions of the complete system are

$$\psi_i=\exp(i\vec{K}_i\cdot\vec{R}_T)\phi_i(\vec{r}_T)\,,$$
$$\psi_f=\exp(i\vec{K}_f\cdot\vec{R}_P)\phi_f(\vec{r}_P)\,,$$

respectively. The interactions of the electron with P and T are, respectively, $V_{Pe}\equiv-Z_Pe^2/r_P$ and $V_{Te}\equiv-Z_Te^2/r_T$. The interaction between P and T is $V_{PT}\equiv Z_PZ_Te^2/R$. The perturbations in the entrance and exit channels are, respectively, $V_i\equiv V_{Pe}+V_{PT}$ and $V_f\equiv V_{Te}+V_{PT}$. The scattering amplitude for the transition $i\to f$ is $A=A_1+A_2$ where

$$A_1\equiv\langle\psi_f|V_i|\psi_i\rangle=\langle\psi_f|V_f|\psi_i\rangle$$

and

$$A_2\equiv\langle\psi_f|V_fG^+V_i|\psi_i\rangle\,,$$

where G^+ is the full Green's function for the system with energy $E+i\eta$, where η is positive but infinitesimal. If H_0 denotes the Hamiltonian obtained by excluding all interactions,

$$G^+\equiv 1/(E+i\eta-H_0-V_i-V_{Te})\,.$$

We approximate G^+ by the Coulomb Green's function G_c^+ which differs from G^+ by the omission of V_i; thus

$$G_c^+\equiv 1/(E+i\eta-H_0-V_{Te})\,.$$

The corresponding approximation to A_2 is

$$A_{2c}\equiv\langle\psi_f|V_fG_c^+V_i|\psi_i\rangle\,.$$

Since the interaction V_{PT} will be dropped (see Sec. IV) we are interested in calculating

$$I_{2c}\equiv\langle\psi_f|V_{Te}G_c^+V_{Pe}|\psi_i\rangle\,.$$

In the next section I_{2c} is reduced to a three-dimensional integral which, with some approximations, is reduced further to a one-dimensional integral.

III. ANALYSIS

In this section we set $\hbar=e=1$ for notational simplicity. We have

$$I_{2c}=\langle\psi_f|V_{Te}|\psi_i^{(1)}\rangle\,,\tag{3.1}$$

where

$$|\psi_i^{(1)}\rangle=G_c^+V_{Pe}|\psi_i\rangle\,.\tag{3.2}$$

Note that

$$(E+i\eta-H_0-V_{Te})|\psi_i^{(1)}\rangle=V_{Pe}|\psi_i\rangle\,.\tag{3.3}$$

We write V_{Pe} in terms of its Fourier transform:

$$V_{Pe}=-\frac{Z_P}{2\pi^2}\int\frac{d^3s}{s^2}e^{i\vec{s}\cdot(\alpha\vec{r}_T-\vec{R}_T)}\,.\tag{3.4}$$

We assume the initial state is the $1s$ state. Writing

$$\phi_i(\vec{r}_T)=N_1e^{-\mu_1r_T}\,,\tag{3.5}$$

where

$$N_1=(Z_T\alpha m)^{3/2}/\pi^{1/2}\,,$$

and where for the moment we leave μ_1 arbitrary but later set $\mu_1=Z_T\alpha m$, we have from Eqs. (3.3)–(3.5),

$$(E+i\eta-H_0-V_{Te})\psi_i^{(1)}(\vec{r}_T,\vec{R}_T)$$
$$=\frac{-Z_PN_1}{2\pi^2}\int\frac{d^3s}{s^2}e^{i\vec{s}\cdot(\alpha\vec{r}_T-\vec{R}_T)-\mu_1r_T+i\vec{K}_i\cdot\vec{R}_T}\,.\tag{3.6}$$

We now express the $\vec{R}_T$ dependence of $\psi_i^{(1)}(\vec{r}_T,\vec{R}_T)$ as a Fourier transform:

$$\psi_i^{(1)}(\vec{r}_T,\vec{R}_T)=\int d^3s\,e^{-i(\vec{s}-\vec{K}_i)\cdot\vec{R}}\tilde{\psi}_i^{(1)}(\vec{r}_T,\vec{s})\,.\tag{3.7}$$

Substituting the right-hand side of Eq. (3.7) into the left-hand side of Eq. (3.6) we find

$$\tilde{\psi}_i^{(1)}(\vec{r}_T,\vec{s})=-(Z_PN_1/2\pi^2s^2)\chi(\vec{q},\vec{r}_T)\,,\tag{3.8}$$

where $\vec{q}=\alpha\vec{s}$ and where

$$\left(-\frac{1}{2\alpha m}\nabla_{\vec{r}}^2-Z_T/r-\mathcal{E}\right)\chi(\vec{q},\vec{r})=-e^{i\vec{q}\cdot\vec{r}-\mu_1r}\,,\tag{3.9}$$
$$\mathcal{E}=E+i\eta-(1/2\nu_i)(\vec{q}/\alpha-\vec{K}_i)^2\,.\tag{3.10}$$

Combining Eqs. (3.1), (3.7), and (3.8), and writing

$$\phi_f(\vec{r}_P) = \left(\frac{1}{2\pi}\right)^{3/2} \int d^3p\, \tilde{\phi}_f(\vec{p}) e^{i\vec{p}\cdot(\alpha\vec{r}_T - \vec{R}_T)}, \quad (3.11)$$

where

$$\tilde{\phi}_f(\vec{p}) = \left(\frac{1}{2\pi}\right)^{3/2} \int d^3r\, \phi_f(\vec{r}) e^{-i\vec{p}\cdot\vec{r}}, \quad (3.12)$$

we obtain

$$I_{2c} = \frac{2^{1/2} Z_T Z_P N_1}{\pi^{1/2}} \int \frac{d^3q}{q^2} \tilde{\phi}_f^*(\vec{q}/\alpha + \vec{K}) Y(\vec{q}), \quad (3.13)$$

$$Y(\vec{q}) = \frac{1}{\alpha} \int \frac{d^3r}{r} e^{i(\vec{J}-\vec{q})\cdot\vec{r}} \chi(\vec{q}, \vec{r}). \quad (3.14)$$

Kelsey and Macek[3] have shown that

$$Y(\vec{q}) = 8\pi X m \left(\frac{ie^{i\pi\tau}}{\sin\pi\tau}\right) \frac{\partial}{\partial\mu_1} \times \int_C d\rho \frac{\rho^{-\tau}}{D_1 D_2 - 2(E_1E_2 - 4X^2\vec{p}_1\cdot\vec{p}_2)\rho + F_1F_2\rho^2}, \quad (3.15)$$

where with $i = 1$ or 2 and with $\mu_2 = 0$,

$$D_i = (X+\mu_i)^2 + p_i^2, \quad (3.16a)$$

$$E_i = -\mu_i^2 - p_i^2 + X^2, \quad (3.16b)$$

$$F_i = (X-\mu_i)^2 + p_i^2, \quad (3.16c)$$

$$X = (-2\alpha m \mathcal{E})^{1/2}, \quad (3.16d)$$

$$\tau = Z_T \alpha m / X, \quad (3.16e)$$

$$\vec{p}_1 = \vec{q}, \quad \vec{p}_2 = \vec{J} - \vec{q}; \quad (3.16f)$$

the contour C starts at $\rho = 1 + i\eta$, where the phase of ρ is zero, and terminates at $\rho = 1 - i\eta$ after encircling the origin once in such a way as to enclose no singularity of the integrand other than the one at the origin.

With $\vec{v}$ along the polar axis, the integration over the azimuthal angle of $\vec{q}$ can be performed in Eq. (3.13) if $\tilde{\phi}_f(\vec{s})$ is isotropic in $\vec{s}$; this leaves a three-dimensional integral to be evaluated. Note that setting $\tau = 0$ is equivalent to replacing G_c^+ by the Green's function for three noninteracting particles.

We now neglect corrections of order m/M_T and m/M_P. We have

$$\vec{K} + \vec{J} + m\vec{v} = 0, \quad (3.17)$$

$$\vec{v}\cdot\vec{K} = -\tfrac{1}{2}mv^2 + \epsilon_i - \epsilon_f, \quad (3.18)$$

$$K^2 + 2m\epsilon_i = J^2 + 2m\epsilon_f. \quad (3.19)$$

Defining

$$\vec{p} \equiv \vec{q} + \vec{K},$$

Eqs. (3.10) and (3.13) become

$$\mathcal{E} = \tfrac{1}{2}mv^2 + \vec{v}\cdot\vec{p} + \epsilon_f + i\eta, \quad (3.20)$$

$$I_{2c} = 2^{1/2} \frac{Z_T Z_P N_1}{\pi^{1/2}} \int \frac{d^3p}{|\vec{p} - \vec{K}|^2} \tilde{\phi}_f^*(\vec{p}) Y(\vec{q}). \quad (3.21)$$

Equations (3.16d)–(3.16f) become

$$X = (-2m\mathcal{E})^{1/2}, \quad (3.22a)$$

$$\tau = Z_T m / X, \quad (3.22b)$$

$$\vec{p}_1 = \vec{p} - \vec{K}, \quad \vec{p}_2 = -\vec{p} - m\vec{v}. \quad (3.22c)$$

To proceed further we assume that $v \gg Z_P$ and that $Z_T \gg Z_P$. Since the presence of $\tilde{\phi}_f^*(\vec{p})$ in Eq. (3.21) restricts the significant values of $\vec{p}$ to $|\vec{p}| \lesssim mZ_P$, we have

$$I_{2c} \approx 2^{1/2} \frac{Z_T Z_P N_1}{\pi^{1/2} K^2} \int d^3p\, \tilde{\phi}_f^*(\vec{p}) Y(\vec{q}), \quad (3.23)$$

$$D_2 = F_2 = Z_P^2 + p^2, \quad (3.24)$$

$$D_1 \approx (X+\mu_1)^2 + K^2, \quad (3.25)$$

$$F_1 \approx (X-\mu_1)^2 + K^2, \quad (3.26)$$

$$E_1E_2 - 4X^2\vec{p}_1\cdot\vec{p}_2 \approx 2(mv)^2(J^2 + \mu_1^2), \quad (3.27)$$

$$X \approx -imv, \quad (3.28)$$

$$\tau \approx iZ_T/v. \quad (3.29)$$

Since τ is now pure imaginary, we can write

$$\left(\frac{ie^{i\pi\tau}}{\sin\pi\tau}\right) \int_C d\rho \cdots = 2\int_0^1 d\rho \cdots. \quad (3.30)$$

With regard to the denominator in the integrand of Eq. (3.15), we see that the coefficient of ρ is much larger than the coefficient F_1F_2 of ρ^2. Since ρ varies from 0 to 1 we could drop the term in ρ^2 with little error, but we did in fact retain this term in our calculation. The constant term D_1D_2 in the denominator is also much smaller than the coefficient of ρ, but this constant term cannot be dropped for otherwise the integrand would have a pole at $\rho = 0$.

With these approximations $Y(\vec{q})$ is isotropic in $\vec{p}$ and the integration over $\vec{p}$ in Eq. (3.23) can be readily performed. In fact, writing

$$I_{2c} \approx \frac{\partial}{\partial\mu_1} \int_0^1 d\rho \int d^3p\, \frac{a\tilde{\phi}^*(\vec{p})}{b^2 + p^2}, \quad (3.31)$$

where a and b depend on μ_1 and ρ, and writing

$$\frac{1}{b^2+p^2} = \frac{1}{4\pi} \int \frac{d^3r}{r} e^{i\vec{p}\cdot\vec{r} - br}, \quad (3.32)$$

we have

$$I_{2c} \approx \left(\frac{\pi}{2}\right)^{1/2} \frac{\partial}{\partial\mu_1} \int_0^1 d\rho\, a \int \frac{d^3r}{r} \phi_f^*(\vec{r}) e^{-br}; \quad (3.33)$$

the integration over $\vec{r}$ is straightforward to perform. Note, however, that if $\phi_f(\vec{r})$ is not isotropic in $\vec{r}$, the right-hand side of Eq. (3.33) is identically

zero from the angular integration over $\vec{r}$; our approximations and therefore inapplicable to final states other than s states. Evidently the cross section for capture to the $2p$ state is significantly smaller than that for capture to the $1s$ state when $Z_T \gg Z_P$ and $v \gg Z_P$. To obtain a nonzero estimate of I_{2c} when the final state is not isotropic we replace Eqs. (3.25)–(3.29) by (where $\hat{v} = \vec{v}/v$)

$$D_1 \approx (\mu_1 - imv)^2 + K^2 + 2\vec{p}\cdot(\vec{J} - i\mu_1\hat{v}), \tag{3.25'}$$

$$F_1 \approx (imv + \mu_1)^2 + K^2 + 2\vec{p}\cdot(\vec{J} - i\mu_1\hat{v}), \tag{3.26'}$$

$$E_1E_2 - 4X^2\vec{p}_1\cdot\vec{p}_2 \approx 2(J^2+\mu_1^2)[(mv)^2 + 2m\vec{v}\cdot\vec{p}], \tag{3.27'}$$

$$X \approx -i(mv + \hat{v}\cdot\vec{p}), \tag{3.28'}$$

$$\tau \approx iZ_T m/(mv + \hat{v}\cdot\vec{p}). \tag{3.29'}$$

However, the integration over $\vec{p}$ is now much more difficult to perform.

The reason that capture occurs predominantly to s states when $Z_T \gg Z_P$ and $v \gg Z_P$ is the following: In order to be captured the electron must acquire during the collision a laboratory velocity that differs from the projectile velocity $\vec{v}$ by at most of the order of the final characteristic orbital speed Z_P. Since $v \gg Z_P$ the projectile P, which is barely deflected during the collision, must penetrate the target electron cloud in order to impart the necessary velocity to the electron. Since the characteristic radius of the target electron cloud is $1/Z_T$ the electron must emerge from the collision within a distance of order $1/Z_T$ of P. The final orbital angular momentum of the electron relative to P is therefore no more than the order of Z_P/Z_T. Hence if $Z_P/Z_T \ll 1$ the electron is captured primarily into s states.

IV. RESULTS AND DISCUSSION

With corrections of order m/M_T and m/M_P neglected, the cross section for electron capture is

$$\sigma = (2\pi\hbar^2v^2)^{-1}\int_0^\infty |A|^2 K_\perp dK_\perp, \tag{4.1}$$

where

$$K_\perp = (K^2 - K_\parallel^2)^{1/2}$$

with

$$K_\parallel = -mv/2\hbar - (\epsilon_f - \epsilon_i)/v\hbar. \tag{4.2}$$

As first pointed out by Wick,[4] when corrections of order m/M_T and m/M_P are neglected the value of σ is independent of whether or not the internuclear potential V_{PT} is included in the Hamiltonian of the system. We exclude V_{PT} from the Hamiltonian since its inclusion would yield a spurious contribution to the cross section obtained by truncating the Born expansion of A. The first Born cross section σ_1 is then defined by approximating A in Eq. (4.1) by I_1 where

$$I_1 \equiv \langle\psi_f|V_{Pe}|\psi_i\rangle = \langle\psi_f|V_{Te}|\psi\rangle. \tag{4.3}$$

The second Born cross sections σ_{2c} and σ_{20} are defined by approximating A by $I_1 + I_{2c}$ and by $I_1 + I_{20}$, respectively, where

$$I_{20} \equiv \langle\psi_f|V_{Te}G_0^+V_{Pe}|\psi_i\rangle, \tag{4.4}$$

and where $G_0^+ \equiv 1/(E + i\eta - H_0)$ is the free Green's function. The cross section σ_s is defined by approximating A by $I_1^2/(I_1 - I_{2c})$; this approximation follows from the Schwinger variational principle.[5]

We calculated the cross sections for $1s \to 1s$ capture for various values of E and Z_T with $Z_P = 1$. Some results are shown in Table I. We calculated σ_{2c} and σ_s by using the peaking approximation described in the preceding section. We calculated σ_{20} by setting $\tau = 0$ and using the same peaking approximation. In Ref. 2, σ_{20} was calculated by using a less restrictive peaking approximation which is valid under the single condition $\hbar v/e^2 \gg Z_P$. The agreement between the present values of σ_{20} and those reported in Ref. 2 is rather good; the discrepancy is about 15% or less. This indicates that the approximations used here are reasonable.

We see from Table I that σ_{2c} is very much smaller than σ_{20} when $\hbar v/e^2 \gg Z_P$ and $\hbar v/e^2 \lesssim Z_T$. In fact for v in this range σ_{2c} does not differ greatly from σ_1. Only when $\hbar v/e^2 \gg Z_T$, Z_P are σ_{2c} and σ_{20} similar in magnitude. The terms I_{20} and I_{2c} each correspond to a double-scattering mechanism in which the electron undergoes two

TABLE I. Electron capture cross section in units of πa_0^2 for various values of the projectile laboratory energy $E_{\rm lab}$ and target atomic number Z_T. The projectile atomic number Z_P is unity and the initial and final states are both $1s$ states. The notation for the cross sections is σ_1, first Born; σ_{2c}, second Born with Coulomb Green's function; σ_{20}, second Born with free Green's function; σ_s, cross section obtained from Schwinger variational principle. A number in parentheses is the power of ten by which the preceding number should be multiplied.

$E_{\rm lab}$ (MeV/amu)	Z_T	σ_1	σ_{2c}	σ_{20}	σ_s
2.5	10	0.51(−5)	0.34(−5)	0.84(−4)	0.67(−6)
2.5	20	0.17(−7)	0.32(−7)	0.14(−5)	0.18(−8)
5.0	10	0.14(−5)	0.84(−6)	0.14(−4)	0.20(−6)
5.0	20	0.45(−7)	0.53(−7)	0.20(−5)	0.33(−7)
10.0	10	0.14(−6)	0.64(−7)	0.83(−6)	0.23(−7)
10.0	20	0.40(−7)	0.23(−7)	0.10(−5)	0.11(−7)

collisions, the first with P and the second with T. This mechanism was originally considered within the framework of classical mechanics by Thomas.[6] The propagation of the electron between the two collisions is described by G_0 in I_{20} and by G_c in I_{2c}. Thus in I_{20} the electron propagates freely between collisions whereas in I_{2c} it propagates in the Coulomb field of T. Now if $\hbar v/e^2 \gg Z_P$ and there is to be a significant probability of capture the electron must emerge from the second collision with a velocity nearly equal to that of P. The velocity of P is almost constant and equal to $\vec{v}$ in the laboratory frame. Since $m/M_T \ll 1$ the second collision is almost elastic in the laboratory frame, and therefore in this frame the electron must propagate between collisions with an energy roughly equal to $\frac{1}{2}mv^2$. Since the motion of an electron with energy $\frac{1}{2}mv^2$ in the field of a nucleus of charge $Z_T e$ is very different from the motion of a free electron when $\hbar v/e^2 \lesssim Z_T$, it is not surprising that I_{20} and I_{2c} differ substantially when v is in this range.

To gain further insight into the difference between I_{20} and I_{2c} we make the impact parameter approximation and write $\vec{R}_T = \vec{b} + \vec{v}t$ where $\vec{b}$ is the impact parameter and t is the time. We define $\xi_c(\vec{r}_T, t)$ by

$$\psi^{(1)}(\vec{r}_T, t) \equiv e^{i\vec{K}_i \cdot \vec{R}_T} \xi_c(\vec{r}_T, t),$$

so that from Eqs. (3.7) and (3.8) we have (with $\hbar = e = 1$)

$$\xi_c(\vec{r}_T, t) = -\frac{Z_P N_1}{2\pi^2} \int \frac{d^3s}{s^2} e^{-i\vec{s}\cdot(\vec{b}+\vec{v}t)} \chi(\vec{s}, \vec{r}_T). \tag{4.5}$$

$\xi_c(\vec{r}_T, t)$ is the first-order correction to the time-dependent electron wave function. The absolute square of the sum of $\phi_i(\vec{r}_T)$ and $\xi_c(\vec{r}_T, t)$ gives the time-dependent charge distribution which evolves during the course of the collision.[7] $\xi_c(\vec{r}_T, t)$ can be expanded in terms of the eigenstates of the "atom" $(e+T)$; the expansion coefficients are, in the limit $t \to \infty$, the first Born amplitudes for direct excitation and ionization (into Coulomb waves) of $(e+T)$. Since the first Born approximation for direct excitation and ionization (into Coulomb waves) in fast asymmetric collisions is reasonably well-founded,[8] $\xi_c(\vec{r}_T, t)$ is expected to give a good description of the overall time-dependent charge distribution. The subscript c on ξ_c emphasizes that ξ_c contains the Coulomb Green's function. Let $\xi_0(\vec{r}_T, t)$ be defined by replacing G_c by G_0 in ξ_c. If $\xi_0(\vec{r}_T, t)$ is expanded in plane waves, the expansion coefficients are, in the limit $t \to \infty$, the first Born amplitudes for direct ionization of $(e+T)$ into *plane waves*. Now if the speed v_e of the ejected electron is small, that is, if $v_e \lesssim Z_T e^2/\hbar$, the first Born amplitude for ejection into a plane wave is a poor estimate of the exact ionization amplitude and greatly exceeds the first Born amplitude for ejection into a Coulomb wave.[9] Therefore $\xi_0(\vec{r}_T, t)$ is expected to give a poor description of the time-dependent charge distribution, at least for those components with $v_e \lesssim Z_T e^2/\hbar$.

Now I_{20} and I_{2c} are obtained by projecting $e^{i\vec{K}_f \cdot \vec{R}_T} \xi_0$ and $e^{i\vec{K}_i \cdot \vec{R}_T} \xi_c$, respectively, onto $\psi_f V_{Te}$. We have

$$\psi_f = e^{i\vec{K}_f \cdot \vec{R}_P} \phi_f = e^{i\beta\vec{K}_f \cdot \vec{R}_T + i(1-\alpha\beta)\vec{K}_f \cdot \vec{r}_T} \phi_f$$

$$\approx e^{im\vec{v}\cdot\vec{r}_T} e^{i\beta\vec{K}_f \cdot \vec{R}_T} \phi_f,$$

where in the last step we have used $(1-\alpha\beta)\vec{K}_f \approx m\vec{v}$ since m/M_T, $m/M_P \ll 1$. In momentum space, only the momentum components of $\phi_f V_{Te}$ with momentum $\lesssim Z_P m e^2/\hbar$ are appreciable. Since $\hbar v/e^2 \gg Z_P$ it is clear that the projection picks out mainly those components of ξ_0 and ξ_c corresponding to the electron being ejected with velocity close to $\vec{v}$. Therefore if $\hbar v/e^2 \lesssim Z_T$ we expect I_{20} to be larger than I_{2c}.

We note, looking at the results in Table I, that σ_s is considerably smaller than σ_{2c}. However, the Schwinger variational principle does not seem to provide a sensible approximation for electron capture since it cannot yield the proper asymptotic form $A \approx I_{20}$ when $\hbar v/e^2 \gg Z_T, Z_P$.

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APPENDIX

We now show for $1s \to 1s$ capture that if $v \gg Z_T \gg Z_P$ the matrix element I_{2c} approaches I_{20}. This provides a check on our approximations. For notational simplicity we set $\hbar = e = m = 1$. I_{20} has the asymptotic form[2]

$$I_{20} \approx 2^5\pi (Z_T Z_P)^{5/2} K^{-4} (v^2 - K^2 + i2Z_T v)^{-1}, \tag{A1}$$

when $v \gg Z_T \gg Z_P$.

We neglect the term $F_1 F_2 \rho^2$ in the denominator of the integrand of Eq. (3.15), we use the approxi-

mations given by Eqs. (3.25)–(3.28), and we set $\tau = 0$ after using Eq. (3.30). We obtain

$$Y(\tilde{q}) \approx -16\pi i v \frac{\partial}{\partial \mu_1} \int_0^1 d\rho \frac{1}{c + d\rho}, \tag{A2}$$

where

$$c = [(\mu_1 - iv)^2 + K^2] D_2, \tag{A3}$$

$$d = -4v^2(J^2 + \mu_1^2). \tag{A4}$$

Performing the differentiation in Eq. (A2), we obtain

$$Y(\tilde{q}) \approx 32\pi i v \int_0^1 d\rho \frac{(\mu_1 - iv)D_2 - 4v^2\mu_1\rho}{(c + d\rho)^2}. \tag{A5}$$

The integration over ρ in Eq. (A5) is straightforward. Setting $\mu_1 = Z_T$ and dropping corrections that are negligible when $v \gg Z_T \gg Z_P$ we obtain (noting $J^2 \approx K^2$)

$$Y(\tilde{q}) \approx \frac{8\pi}{K^2(v^2 - K^2 + i2Z_T v)}; \tag{A6}$$

the term $i2Z_T v$ in the denominator is not neglibible compared to the term $v^2 - K^2$ since we may have $K = v$. Note that asymptotically $Y(\tilde{q})$ is independent of $\tilde{p}$. Combining Eqs. (3.23) and (A6), and using

$$\int \tilde{\phi}^*(\tilde{p}) d^3p = (2\pi)^{3/2} \phi_f^*(0), \tag{A7}$$

we find that I_{2c} is asymptotically equal to the right-hand side of Eq. (A1), as we had set out to prove.

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[1] K. Dettmann, Springer Tracts Mod. Phys. 58, 119 (1971); R. Shakeshaft and L. Spruch, Rev. Mod. Phys. 51, 369 (1979).

[2] R. Shakeshaft, Phys. Rev. Lett. 44, 442 (1980).

[3] E. J. Kelsey and J. Macek, J. Math. Phys. 17, 1182 (1976).

[4] See the footnote on p. 359 of the paper by J. D. Jackson and H. Schiff, Phys. Rev. 89, 359 (1953).

[5] See, e.g., the first paper of Ref. 1.

[6] L. H. Thomas, Proc. R. Soc. London 114, 561 (1927).

[7] Maps of the time-dependent charge distribution in a proton-hydrogen atom collision may be seen in R. Shakeshaft, Phys. Rev. A 18, 1930 (1978).

[8] N. F. Mott and H. S. W. Massey, *Theory of Atomic Collisions*, 3rd ed. (Oxford University, London, 1965), p. 615; M. E. Rudd and J. H. Macek, Case Stud. At. Phys. 3, 49 (1972), particularly pp. 122–124.

[9] For example, we calculated the doubly differential cross section $d^2\sigma/d\Omega_e dv_e$ for an electron to be ejected into the forward direction by a proton incident with a laboratory energy of 300 keV on a hydrogen atom. The value of $d^2\sigma/d\Omega_e dv_e$ calculated in the first Born approximation using plane waves exceeds the value calculated using Coulomb waves by factors of about 70 and 3 when the electron is ejected with laboratory energies of 10 and 100 eV, respectively.