Relativistic eikonal theory of electron capture

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The eikonal theory of electron capture by relativistic projectiles is developed. It is shown that as long as the electron spin is not measured, a density-matrix formalism can greatly simplify the calculation. The exact eikonal cross section is expressed in terms of two-dimensional integrals. For $1s$-$1s$ capture an approximate closed-form expression valid for not too high nuclear charges is also given. This form explicitly displays contributions from magnetic capture and from relativistic modifications of the electron orbits. At each stage of the development the corresponding Oppenheimer-Brinkman-Kramers (OBK) result can be retrieved as a special case. It is concluded that the multiple-scattering contributions described by the eikonal approach are crucial in reducing the calculated cross section significantly below the OBK and second-Born-approximation values. In this way, good agreement with experimental data is obtained.

I. INTRODUCTION

With the currently developing possibilities to extract nonradiative electron-capture cross sections[1] from experimental data[2] collected in relativistic heavy-ion collisions it is timely now to extend the understanding of capture processes into the relativistic regime. Earlier theoretical work[3–7] in this field has, perhaps, been motivated not so much by the pressure of existing experimental data as by the desire to put the structural examination of electron capture at very high velocities on a more realistic basis. Indeed, cross-section studies at asymptotic velocities[8] have played an eminent role in recognizing the unique behavior of the double-scattering (Thomas) mechanism in nonrelativistic capture theories.

It is natural, therefore, that most of the pioneering work on relativistic capture has been based on the first-order Born, or Oppenheimer-Brinkman-Kramers (OBK), approximation.[3–5] Unlike the nonrelativistic OBK (Ref. 9) in which the cross section falls off as E^{-6} with increasing energy E the relativistic OBK (Refs. 3–5) or impulse[6] approximations yield an asymptotic decay as E^{-1}. This feature remains unchanged when relativistic second-Born-approximation terms are included.[7] While for nonrelativistic capture the double-scattering mechanism with an $E^{-11/2}$ dependence is asymptotically dominant[8,9] it simply leads to a reduction of the total cross section in the relativistic case[7] and can be identified[7] only by the characteristic Thomas peak in the differential cross section.

Although the structural behavior of the cross section is of great theoretical significance it is necessary also to compare calculated values with experimental data which are now emerging.[1,2] And here it turns out[1,10] that, for example, calculated[5] OBK cross sections for 1050-MeV/amu Ne on targets with charge numbers between 13 and 92 are almost a factor of 10 too large. Similar conclusions hold for other systems. Since also the inclusion of second-order Born terms[7] does not bring predictions close to the data, it is mandatory to formulate a relativistic multiple-scattering theory.

In the present study we develop a relativistic extension for the eikonal approach[11–16] to electron capture. In doing so we demonstrate, quite generally, that a capture theory using relativistic electron wave functions is conveniently formulated in a density-matrix formalism which from the outset allows for summing or averaging over presently unobservable spin states. It is then unnecessary to separately calculate non-spin-flip and spin-flip transitions[5,7] and hence the calculation is greatly simplified. A brief account of this work, together with a comparison to experimental data, has been given in Ref. 10.

The nonrelativistic eikonal approach[11–16] is a comparatively accessible multiple-scattering theory which renders good overall agreement with experimental data for total[12,14] and state-to-state[13] cross sections in symmetric or near-symmetric collision systems at intermediate velocities. The conceptual basis of the approach has been discussed in some detail,[15,16] and it has been shown that, physically, the prior (post) version of the theory describes a hard collision of the electron with the projectile (target) nucleus followed (preceded) by multiple soft collisions with the target (projectile) nucleus. Not included is that small portion of phase space[15,16] corresponding to hard-hard collisions and giving rise to the elusive Thomas peak[17] and the asymptotic $E^{-11/2}$ dependence of the cross section mentioned before. Thus the eikonal approach while missing an interesting but difficult to observe part of the second-Born-approximation term does include higher-order Born terms albeit in an approximate way. The multiple-scattering contributions included in the eikonal approximation are expected[16] to play a decisive role in an adequate description of the charge transfer mechanism. One can also convince oneself[18] that, within the range of applicability, the eikonal approach gives results very similar (within 10%) to those of the strong potential Born (SPB) approximation[19] for total and forward cross sections. The SPB approximation, while not exactly without difficulties,[20] is considered a reliable starting

point for subsequent approximations.

One may feel confident that a relativistic generalization of the eikonal approach should give realistic estimates for capture cross sections at sufficiently high energies, in particular because the Thomas mechanism does not qualitatively affect[7] the cross-section behavior at high energies.

The plan of the paper is as follows. Starting from a covariant form of the transition amplitude we derive in Sec. II a general cross-section formula expressed in terms of density matrices for initial and final states and in terms of transformation matrices. Subsequently, in Sec. III, we explicitly calculate the density matrices and the resulting cross section for $1s$-$1s$ transitions. With the aid of an αZ expansion, this formula is cast into an approximate closed-form expression in Sec. IV, while in Sec. V we show how to generalize the density-matrix method to arbitrary initial and final states. In Sec. VI we conclude with a discussion of results. Atomic units are used unless explicitly stated otherwise.

II. GENERAL FORMULATION

Consider a collision system consisting of a hydrogenic target (charge Z_T) at rest and a bare projectile (charge Z_P) moving along a rectilinear trajectory $\mathbf{R}=\mathbf{b}+\mathbf{v}t$ with respect to the target nucleus where $\mathbf{v}$ is a constant velocity and $\mathbf{b}$ the impact parameter. Space-time coordinates of the electron are denoted by $\mathbf{r},t$ in the target frame and by $\mathbf{r}',t'$ in the projectile frame. We use atomic units $\hbar=e=m=1$, however, the electron mass m is explicitly displayed when it serves the understanding.

The capture cross section averaged over the initial and summed over the final projections μ,μ' of the electron angular momentum j,j' is given by

$$\sigma_{fi}=\frac{1}{2j+1}\sum_{\mu,\mu'}\int |A_{fi}^{\mu',\mu}(\mathbf{b},v)|^2 d^2b \ . \tag{2.1}$$

Here, in the amplitude A_{fi} for capture (suppressing spin labels for the moment) the perturbation acting on the electron four-current[21] $-i\bar{\psi}\gamma_\nu\psi$ (with $\bar{\psi}=\psi^\dagger\gamma_4$) is the electromagnetic four-potential A_ν. Setting up the final wave function and the four-potential in the projectile frame and subsequently transforming to the laboratory frame we can write the transition amplitude[4-6] in the covariant form

$$A_{fi}=-i\int dt\int d^3r\overline{[S^{-1}\psi_f'(\mathbf{r}_P',t')]}\times[-iS^{-1}\gamma_\nu A_\nu'(\mathbf{r}_P',t')S]\psi_i(\mathbf{r}_T,t) \ , \tag{2.2}$$

where the spinor transform S that transforms from the target frame to the projectile frame is defined by

$$\psi'(\mathbf{r}',t')=S\psi(\mathbf{r},t) \ . \tag{2.3}$$

In the prior form of the theory, the electromagnetic four-potential A_ν is produced by the projectile nucleus. Hence, in the projectile frame, it is simply the instantaneous Coulomb potential. The covariant operator is then identified as

$$-i\gamma_\nu A_\nu'=-\gamma_4\frac{Z_P}{r_P'} \tag{2.4}$$

and subsequently transformed to the target system using[21]

$$S(v)=\left[\frac{\gamma+1}{2}\right]^{1/2}(1-\delta\alpha_z)=S^\dagger(v) \ , \tag{2.5}$$

where $\gamma=(1-v^2/c^2)^{-1/2}$, $\delta=[(\gamma-1)/(\gamma+1)]^{1/2}$, and α_z is the component of the Dirac $\boldsymbol{\alpha}$ matrix in the beam direction. From (2.4) and the relation $\gamma_4 S(v)\gamma_4=S^{-1}(v)=S(-v)$ we see that the electron-projectile interaction in the laboratory system takes the form

$$V_P(\mathbf{r}_p,t)=-\frac{Z_P}{r_P'}\gamma\left[1-\frac{v}{c}\alpha_z\right]=-\frac{Z_P}{r_P'}S^2 \ . \tag{2.6}$$

The term with $(v/c)\alpha_z$ accounts for the Lorentz contraction of the Coulomb field as well as for the induced magnetic interaction. From (2.6) and (2.2) we immediately obtain the simpler form

$$A_{fi}=i\int dt\int d^3r[\psi_f'(\mathbf{r}_P',t')]^\dagger S\frac{Z_P}{r_P'}\psi_i(\mathbf{r}_T,t) \ . \tag{2.7}$$

It now remains to specify the spinor wave functions. In the prior form of the eikonal approach adopted and appropriate for $Z_P\lesssim Z_T$ the initial and final wave functions

$$\psi_i(\mathbf{r}_T,t)=\phi_i(\mathbf{r}_T)e^{-iE_it} \tag{2.8a}$$

and

$$\psi_f'(\mathbf{r}_P',t')=\phi_f'(\mathbf{r}_P')\exp(-iE_ft')\exp\left[-iZ_T'\int_t^\infty\frac{1}{r_T}dt''\right] \tag{2.8b}$$

are expressed by the stationary target and projectile wave functions ϕ_i and ϕ_f', respectively, and the time-dependent phase factors associated with the relativistic energies E_i and E_f. The final wave function is phase distorted by the electron-target interaction integrated from the time of capture to infinity. In the target frame, the interaction is a simple Coulomb potential, and the corresponding target charge is denoted by Z_T' where the prime provides a unique signature for the electron-target interaction in the eikonal phase. It is clear that for $Z_T'=0$ we recover the OBK approximation. The eikonal integral in (2.8b) has to be evaluated with $\mathbf{r}_P'$ kept fixed. This is in line with the condition for the validity of the eikonal approach[15] that the kinetic energy of a free electron traveling with the speed of the projectile is large compared to the larger one of the binding energies in initial or final state, or $\gamma-1\gg 1-(1-\alpha^2Z^2)^{1/2}$ for $1s$-$1s$ capture.

Transforming the final-state time oscillation into the target frame we get[22]

$$\psi_f'(\mathbf{r}_P',t')=\phi_f'(\mathbf{r}_P')\exp[-i\gamma E_f(t-vz_T/c^2)]\times\exp[i\nu\ln(r_T+z_T)] \ , \tag{2.9}$$

where $\nu=\eta Z_T'$ and $\eta=1/v$. At this point, we may easily convince ourselves that in the nonrelativistic limit (energy ϵ_f) the phase describing the time oscillation in the projectile frame

$$\gamma E_f(t-vz_T/c^2)=mc^2t+\epsilon_f t+\tfrac{1}{2}mv^2t-m(\mathbf{v}\cdot\mathbf{r}_T)+\cdots \tag{2.10}$$

consists of an immaterial contribution from the electron mass (which is canceled by the corresponding term from E_i), the nonrelativistic eigenoscillation and the familiar translational factor. With the aim of evaluating (2.7), we use the Gau-Macek representation[23] to rewrite

$$e^{-i\nu\ln(r_T+z_T)}=[\Gamma(i\nu)]^{-1}\int_0^\infty \lambda^{i\nu-1}e^{-\lambda(r_T+z_T)}d\lambda \tag{2.11}$$

and combine the coordinate-dependent exponential within the integrand with the initial wave function to define the Fourier transform $h(\mathbf{p},\lambda)$ through

$$\phi_i(\mathbf{r}_T)e^{-\lambda(r_T+z_T)}=(2\pi)^{-3/2}\Gamma(i\nu)\int h(\mathbf{p},\lambda)e^{-i\mathbf{p}\cdot\mathbf{r}_T}d^3p\ . \tag{2.12}$$

Similarly, for the final-state wave function we introduce the Fourier transform $g(\mathbf{q})$ through

$$\phi_f'(\mathbf{r}_P')\frac{1}{r_P'}=(2\pi)^{-3/2}\int g(\mathbf{q})e^{-i\mathbf{q}\cdot\mathbf{r}_P'}d^3q\ . \tag{2.13}$$

Both g and h are 4-spinors. Now, by combining (2.8) with (2.9), (2.12), and (2.13) one may move all space-time coordinates to the exponents so that these integrations can be readily performed. With $\mathbf{p}=(\mathbf{p}_b,p_z)$ and $\mathbf{q}=(\mathbf{q}_b,q_z)$ Eq. (2.7) immediately leads to the transition amplitude

$$A_{fi}^{\mu'\mu}=i\frac{2\pi\eta Z_P}{\gamma}\int d^2p_b\int d\lambda\, g_{\mu'}^\dagger(\mathbf{p}_b,p_+)Sh_\mu(\mathbf{p}_b,p_-;\lambda)\times\lambda^{i\nu-1}e^{-i\mathbf{p}_b\cdot\mathbf{b}}\ , \tag{2.14}$$

where we have reintroduced the angular momentum components. The longitudinal components of $\mathbf{p}$ and $\mathbf{q}$ take the fixed values

$$p_-=\eta(E_f/\gamma-E_i) \tag{2.15a}$$

and

$$P_g^{\mu'}=g_{\mu'}(\mathbf{p}_b,p_+)g_{\mu'}^\dagger(\mathbf{p}_b,p_+) \tag{2.16b}$$

Owing to its spinor structure, the expression (2.14) is rather involved and the evaluation would have to be repeated for each essentially different combination of μ' and μ. For example, in his $1s$-$1s$ OBK calculation Shakeshaft[4] considers only non-spin-flip transitions while Moiseiwitsch and Stockman[5] separately calculate non-spin-flip and spin-flip cross sections.

A simplification can, however, be achieved by constructing density matrices from the initial and final 4-spinors h and g and by summing over the (currently unobservable) angular momentum projections within each of the density matrices. We hence define

$$P_g=\sum_{\mu'}P_g^{\mu'} \tag{2.16a}$$

with

$$P_g^{\mu'}=g_{\mu'}(\mathbf{p}_b,p_+)g_{\mu'}^\dagger(\mathbf{p}_b,p_+) \tag{2.16b}$$

and, similarly,

$$P_h=\sum_\mu P_h^\mu \tag{2.17a}$$

with

$$P_h^\mu=\int_0^\infty d\lambda\int_0^\infty d\lambda' h_\mu(\mathbf{p}_b,p_-;\lambda)h_\mu^\dagger(\mathbf{p}_b,p_-;\lambda')\lambda^{i\nu-1}\times(\lambda')^{-i\nu-1}\ . \tag{2.17b}$$

It is clear and will become explicit in Sec. III that it is considerably simpler to calculate P_g and P_h than any one of the $P_g^{\mu'}$ or P_h^μ.

We are now ready to insert (2.14) into (2.1), integrating over the impact-parameter plane and introducing the density matrices (2.16) and (2.17). In this way, we obtain the cross section in the compact form

$$\sigma_{fi}=\frac{(2\pi)^4}{2j+1}\frac{\eta^2}{\gamma^2}Z_p^2\int \mathrm{Tr}\{SP_gSP_h\}d^2p_b\ , \tag{2.18}$$

where the integrand is expressed as the trace of a product of four 4×4 matrices. The task is now reduced to constructing the matrices P_g and P_h for each individual case considered. This will be done in the following sections. Owing to axial symmetry, the integration remaining in (2.18) will, in general, be simply a one-dimensional integral.

III. CAPTURE FROM INITIAL $1s_{1/2}$ STATES INTO FINAL $1s_{1/2}$ STATES

The presence of high-momentum components in initial and final states renders $1s$-$1s$ capture the most important case at high collision energies and it is also the only case that has been considered so far within the Born[3–5,7] or impulse[6] approximations. For evaluating (2.18) we first have to set up the appropriate density matrices P_g and P_h.

Starting point is the spinor wave function[21,24,25] for the hydrogenic $1s$ state

$$\phi_\mu(\mathbf{r})=(4\pi)^{-1/2}\begin{bmatrix} g(r)\chi_\mu \\ -if(r)(\boldsymbol{\sigma}\cdot\hat{\mathbf{r}})\chi_\mu\end{bmatrix}, \tag{3.1}$$

where χ_μ with $\mu=\pm\frac{1}{2}$ denotes a Pauli spinor, $\hat{\mathbf{r}}=\mathbf{r}/r$, and the standard radial functions[24] are

$$\begin{aligned} g(r)&=N_g r^{s-1}e^{-Zr}\ ,\\ f(r)&=N_f r^{s-1}e^{-Zr}\ , \end{aligned} \tag{3.2}$$

with $s=[1-(\alpha Z^2)]^{1/2}$, $\alpha=\frac{1}{137}$, and the normalization factors

$$\begin{aligned} N_g&=\frac{(2Z)^{s+1/2}}{[2\Gamma(2s+1)]^{1/2}}(1+s)^{1/2}\ ,\\ N_f&=-\frac{(2Z)^{s+1/2}}{[2\Gamma(2s+1)]^{1/2}}(1-s)^{1/2}\ . \end{aligned} \tag{3.3}$$

The Fourier transform $g_\mu(\mathbf{q})$ is obtained by inverting the defining relation (2.13) and by inserting the partial-wave expansion

$$e^{i\mathbf{q}\cdot\mathbf{r}_P}=4\pi\sum_{l,m}i^l j_l(qr_P)Y_{lm}^*(\hat{\mathbf{r}}_P)Y_{lm}(\hat{\mathbf{q}}) \tag{3.4}$$

of the plane wave. Clearly, only $l=0$ and $l=1$ contribute to the integrals over g and f, respectively, and leave us with radial integrals whose evaluation[26] leads to

$$a(q)=\frac{1}{q}\frac{N_g\Gamma(s_P)}{(Z_P^2+q^2)^{s_P/2}}\sin\left[s_P\tan^{-1}\left[\frac{q}{Z_P}\right]\right] \tag{3.5a}$$

and

$$b(q)=\frac{1}{q^2}\frac{N_f\Gamma(s_P-1)}{(Z_P^2+q^2)^{(s_P-1)/2}}\sin\left[(s_P-1)\tan^{-1}\left[\frac{q}{Z_P}\right]\right]$$
$$-\frac{1}{q}\frac{N_f\Gamma(s_P)}{(Z_P^2+q^2)^{s_P/2}}\cos\left[s_P\tan^{-1}\left[\frac{q}{Z_P}\right]\right]. \tag{3.5b}$$

As a result, we obtain g_μ in a form that closely resembles (3.1) as

$$g_\mu(q)=\frac{1}{\pi\sqrt{2}}\begin{bmatrix}a(q)\chi_\mu\\ b(q)(\boldsymbol{\sigma}\cdot\hat{\mathbf{q}})\chi_\mu\end{bmatrix}. \tag{3.6}$$

Of course, when g_μ is used in (2.14) we have $q^2=p_b^2+p_+^2$ with p_+ given by (2.15b) and (for $1s$-$1s$ transitions) related to p_- via $Z_P^2+p_+^2=Z_T^2+p_-^2$. As (3.6) is made up of Pauli spinors, the spin-dependent density matrix (2.16b)

$$P_g^\mu=\frac{1}{2\pi^2}\begin{bmatrix}a^2\chi_\mu\chi_\mu^\dagger & ab\chi_\mu\chi_\mu^\dagger(\boldsymbol{\sigma}\cdot\hat{\mathbf{q}})\\ ab(\boldsymbol{\sigma}\cdot\hat{\mathbf{q}})\chi_\mu\chi_\mu^\dagger & b^2(\boldsymbol{\sigma}\cdot\hat{\mathbf{q}})\chi_\mu\chi_\mu^\dagger(\boldsymbol{\sigma}\cdot\hat{\mathbf{q}})\end{bmatrix} \tag{3.7}$$

is built from blocks of 2×2 matrices. At this point, it becomes clear how much is gained by first summing over the spin projections μ. Since $\sum_\mu\chi_\mu\chi_\mu^\dagger=1$ is the 2×2 unit matrix we have

$$P_g=\frac{1}{2\pi^2}\begin{bmatrix}a^2 & ab(\boldsymbol{\sigma}\cdot\hat{\mathbf{q}})\\ ab(\boldsymbol{\sigma}\cdot\hat{\mathbf{q}}) & b^2\end{bmatrix}, \tag{3.8}$$

where use has been made of the relation $(\boldsymbol{\sigma}\cdot\mathbf{u})(\boldsymbol{\sigma}\cdot\mathbf{v})=\mathbf{u}\cdot\mathbf{v}+i\boldsymbol{\sigma}\cdot(\mathbf{u}\times\mathbf{v})$ to be employed throughout our further development. If one wants to keep the spin information one may substitute $\chi_\mu\chi_\mu^\dagger=\frac{1}{2}(1\pm\sigma_z)$ for $\mu=\pm\frac{1}{2}$ in (3.7) and subsequently use the same techniques. However, the reduction work—allowing for spin specification in initial and final states—is increased by a significant factor.

The construction of P_h defined by (2.17) proceeds exactly along the same line. Complications arise from the presence of the factor $e^{-\lambda(r_T+z_T)}$ and from the integration over λ. While the radial part of the exponent can be combined with that of the wave function (3.2) the term $e^{-\lambda z_T}$ is absorbed into the plane wave by defining[14] a complex wave vector

$$\mathbf{k}_\lambda=\mathbf{p}+i\lambda\hat{\mathbf{e}}_z=(\mathbf{p}_b;p_-+i\lambda) \tag{3.9}$$

with $k_\lambda^2=p_b^2+p_-^2-\lambda^2+2i\lambda p_-$ and p_- being given by (2.15a). As a result, the quantities $a(q)$, $b(q)$, and $\hat{\mathbf{q}}$ in (3.6) have to be replaced with complex integrals. With the abbreviation $\lambda_\pm=\lambda+Z_T\pm ik_\lambda$ and $s=s_T$ the integrals take the form

$$A_0(\mathbf{p})=N_g\frac{\Gamma(s+1)}{\Gamma(i\nu)}\int_0^\infty\frac{1}{2ik_\lambda}(\lambda_-^{-(s+1)}-\lambda_+^{-(s+1)})\times\lambda^{i\nu-1}d\lambda, \tag{3.10}$$

$$B_m(\mathbf{p})=N_f\frac{\Gamma(s)}{\Gamma(i\nu)}\int_0^\infty\frac{1}{2ik_\lambda^3}(\lambda_-^{-s}-\lambda_+^{-s})\lambda^{i\nu-1+m}d\lambda$$
$$-N_f\frac{\Gamma(s+1)}{\Gamma(i\nu)}\int_0^\infty\frac{1}{2k_\lambda^2}(\lambda_-^{-(s+1)}+\lambda_+^{-(s+1)})\times\lambda^{i\nu-1+m}d\lambda. \tag{3.11}$$

If the integrals B_m with $m=0,1$ are combined to build a vector

$$\mathbf{K}=(B_0\mathbf{p}_b,\ B_0p_-+iB_1) \tag{3.12}$$

the λ integral over the spinor function h_μ defined in (2.12) assumes a structure analogous to (3.6),

$$\int_0^\infty h_\mu(\mathbf{p},\lambda)\lambda^{i\nu-1}d\lambda=\frac{1}{\pi\sqrt{2}}\begin{bmatrix}A_0\chi_\mu\\ (\boldsymbol{\sigma}\cdot\mathbf{K})\chi_\mu\end{bmatrix}. \tag{3.13}$$

The density matrices (2.17) are then obtained as in (3.7) and (3.8). We just give the density matrix summed over spin states

$$P_h=\frac{1}{2\pi^2}\begin{bmatrix}|A_0|^2 & A_0(\boldsymbol{\sigma}\cdot\mathbf{K}^*)\\ (\boldsymbol{\sigma}\cdot\mathbf{K})A_0^* & (\boldsymbol{\sigma}\cdot\mathbf{K})(\boldsymbol{\sigma}\cdot\mathbf{K}^*)\end{bmatrix}. \tag{3.14}$$

This completes the construction of the matrices entering in (2.18). The matrix multiplication now can be easily carried out by using the properties of the Pauli submatrices.

As an intermediate result to be used with $1s_{1/2}$ final and any initial state we give here the matrix product

$$SP_gS=\frac{\gamma+1}{8\pi^4}\begin{bmatrix}m_{11} & m_{12}(\boldsymbol{\sigma}\cdot\hat{\mathbf{q}})+m'_{12}(\boldsymbol{\sigma}\cdot\hat{\mathbf{e}}_z)\\ m_{12}(\boldsymbol{\sigma}\cdot\hat{\mathbf{q}})+m'_{12}(\boldsymbol{\sigma}\cdot\hat{\mathbf{e}}_z) & m_{22}\end{bmatrix} \tag{3.15}$$

with $\hat{\mathbf{q}}=\mathbf{q}/q$, $\hat{\mathbf{e}}_z$ a unit vector in the beam direction, and the coefficients

$$m_{11}=a^2-2\delta ab\hat{q}_z+\delta^2b^2,\quad m_{12}=ab(1-\delta^2),\quad m'_{12}=-\delta(a^2-2\delta ab\hat{q}_z+b^2),\quad m_{22}=\delta^2a^2-2\delta ab\hat{q}_z+b^2. \tag{3.16}$$

Here $\delta=[(\gamma-1)/(\gamma+1)]^{1/2}$, $\hat{q}_z=p_+/q$, and $q=(p_b^2+p_+^2)^{1/2}$. In the final matrix multiplication of (3.15) and (3.14) in (2.18) we only need to consider terms that contribute to the trace. The final result for the cross section for capture of an (unpolarized) $1s$ electron into both possible $1s$ states of the projectile is then obtained as

$$\sigma_{1s\text{-}1s}=2\pi\eta^2 Z_P^2\frac{\gamma+1}{\gamma^2}\int_0^\infty Q(p_b^2)d(p_b^2)\ . \tag{3.17}$$

Here, the integrand is given by

$$\begin{aligned}Q=&m_{11}\,|\,A_0\,|^2\\&+(2m_{12}/q)[\mathrm{Re}(A_0B_0^*)(p_b^2+p_+p_-)+\mathrm{Im}(A_0B_1^*)p_+]\\&+2m'_{12}[\mathrm{Re}(A_0B_0^*)p_-+\mathrm{Im}(A_0B_1^*)]\\&+m_{22}[\,|\,B_0\,|^2(p_b^2+p_-^2)+2\,\mathrm{Im}(B_0B_1^*)p_-+|\,B_1\,|^2]\ .\end{aligned} \tag{3.18}$$

The calculation of the cross section requires the numerical evaluation of the λ integrals in A_0,B_0,B_1 and the additional one-dimensional integration over p_b^2. The results of such calculations have been given and discussed in an earlier publication.[10]

Just for completeness we also give here the capture cross section in the OBK approximation obtained for $Z_T'\to 0$ or $v\to 0$. Recalculation of P_h shows that in (3.17) we simply have to substitute the modified integrand

$$\begin{aligned}Q^{\mathrm{OBK}}=&m_{11}\bar{a}^2+\frac{2m_{12}}{pq}\bar{a}\bar{b}(p_b^2+p_+p_-)\\&+\frac{2m'_{12}}{p}\bar{a}\bar{b}p_-+m_{22}\bar{b}^2\ .\end{aligned} \tag{3.19}$$

Here, the m_{ij} are the same [Eqs. (3.16)] as before, $q=(p_b^2+p_+^2)^{1/2}$, $p=(p_b^2+p_-^2)^{1/2}$, and the quantities $\bar{a},\bar{b}$ result from a,b of (3.5) by the replacements $Z_P\to Z_T$, $q\to p$, $s_P\to s_T+1$. The cross section is structurally similar and numerically identical[10] to the result obtained by adding the non-spin-flip and spin-flip cross sections of Moiseiwitsch and Stockman.[5] In Sec. IV we give a direct comparison of the more transparent approximate forms of both the OBK and eikonal results.

IV. APPROXIMATION ANALYTICAL EXPRESSION FOR THE $1s$-$1s$ CROSS SECTION

While it is not difficult to evaluate the cross-section formula (3.17) numerically, it is instructive to give an approximate expression and to discuss it in some detail. Note that our treatment includes two kinds of relativistic effects, namely the relativistic kinematics of the projectile motion and the relativistic motion of the electron in its initial and final atomic orbits. Compared to the nonrelativistic case, the latter has two important consequences. (1) The electron orbitals and their binding energies are modified in a Z-dependent manner. (2) The electron acquires a Dirac magnetic moment which in turn interacts with the induced magnetic field arising from the Lorentz transform of the static Coulomb field of target and projectile. The occurrence of a Dirac magnetic moment for the electron is, of course, independent of the binding nuclear charge, and hence magnetic capture will have the same charge dependence as Coulomb capture.

In order to study corrections to the kinematically determined capture cross section, we expand the electronic wave functions in powers of $\alpha Z_{P,T}\ll 1$ keeping only the leading terms and assuming that high-energy approximations can be applied to these correction terms.[5] This means that (within the correction terms) $p_\pm^2\simeq(137\delta)^2\gg Z_{P,T}^2$ and $\tan^{-1}(q/Z_P)\simeq\pi/2$ in (3.5). Correspondingly, in (3.10) and (3.11), we assume that contributions to the integrals arise mainly from values of $\lambda\ll 137$. Using again $\eta=1/v$, $\delta=[(\gamma-1)/(\gamma+1)]^{1/2}$, and substituting $\nu=\eta Z_T'$ (where $Z_T'=0$ for the OBK and $Z_T'=Z_T$ for the one-electron eikonal approximation) we derive the result[10]

$$\begin{aligned}\sigma_{1s\text{-}1s}^{\mathrm{eik}}=&\frac{2^8\pi Z_P^5Z_T^5}{5v^2(Z_T^2+p_-^2)^5}\frac{\gamma+1}{2\gamma^2}\frac{\pi\eta Z_T'}{\sinh(\pi\eta Z_T')}\\&\times e^{-2\eta Z_T'\tan^{-1}(-p_-/Z_T)}(S_{\mathrm{eik}}+S_{\mathrm{magn}}+S_{\mathrm{orb}})\end{aligned} \tag{4.1}$$

with

$$S_{\mathrm{eik}}=1+\frac{5}{4}\eta\frac{Z_T'}{Z_T}p_-+\frac{5}{12}\eta^2\frac{(Z_T')^2}{Z_T^2}p_-^2+\frac{1}{6}\eta^2(Z_T')^2\ , \tag{4.2a}$$

$$S_{\mathrm{magn}}=-\delta^2+\frac{5}{16}\delta^4+\frac{5}{8}\delta^2\frac{\gamma}{\gamma+1}\frac{Z_T'}{Z_T}+\frac{1}{4}\delta^2\eta^2(Z_T')^2+\frac{5}{48}\delta^4\eta^2(Z_T')^2\ , \tag{4.2b}$$

$$\begin{aligned}S_{\mathrm{orb}}=&\frac{5\pi}{18}\delta\alpha(Z_P+Z_T)-\frac{5\pi}{36}\delta^3\alpha(Z_P+Z_T)\\&-\frac{5}{8}\delta\alpha Z_T\eta Z_T'(1-\tfrac{1}{2}\delta^2)-\frac{5\pi}{18}\delta\frac{\gamma}{\gamma+1}\alpha Z_P\frac{Z_T'}{Z_T}\\&+\frac{5\pi}{28}\delta\left[\frac{\gamma}{\gamma+1}\right]^2\alpha Z_P\frac{(Z_T')^2}{Z_T^2}\\&-\frac{5\pi}{28}\delta\frac{\gamma}{\gamma+1}\alpha(Z_P+Z_T-\delta^2Z_P)\frac{Z_T'}{Z_T}\ .\end{aligned} \tag{4.2c}$$

This final approximate expression embraces a number of limiting cases which we are now going to discuss. (1) If we only keep S_{eik} in (4.1), we obtain the exact eikonal cross section for relativistic kinematics but nonrelativistic electron wave functions. (2) If, furthermore, we let $\gamma\to 1$ and use the nonrelativistic limit $p_-^{\mathrm{nr}}=\epsilon\eta-\frac{1}{2}v$ where $\epsilon=-\frac{1}{2}(Z_P^2-Z_T^2)$ we recover the nonrelativistic eikonal cross section.[12] (3) If, in addition, we let $Z_T'\to 0$, (4.1) collapses to the nonrelativistic OBK cross section.[9] (4) By using the full expression (4.1) but with $Z_T'\to 0$, so that $S_{\mathrm{eik}}\to 1$ and S_{magn} and S_{orb} each reduce to the first two terms, we retrieve the approximate relativistic OBK results (summed over non-spin-flip and spin flip) of Moiseiwitsch and Stockman[5] within the approximation $Z_T^2\ll p_-^2$ used both in Ref. 5 and here for the correction

terms. (5) The term S_{magn} does not depend on the binding nuclear charges (Z_T' represents a final-state interaction) and hence is interpreted as a magnetic contribution to capture. It may be worthwhile to note that, according to Ref. 5, the term $-\delta^2$ is entirely due to non-spin-flip whereas $\frac{5}{16}\delta^4$ is $\frac{1}{4}$ non-spin-flip and $\frac{1}{16}$ spin flip. (6) S_{orb} is composed of terms that explicitly include αZ_P or αZ_T and hence are interpreted as correction terms arising from a relativistic modification of the electronic orbitals. While the OBK contribution is symmetric with respect to $Z_P \leftrightarrow Z_T$ owing to the post-prior symmetry of the theory, the eikonal contribution (with Z_T') is not.[27]

A comparison with the results of an exact numerical evaluation of (3.17) shows[10] that the approximate formula (4.1) is very accurate at small $\alpha Z_{P,T}$ and still for $Z_T=73$ (at $Z_P=10$, $E=1050$ MeV/amu) deviates no more than 15%.

We briefly comment on the asymptotic behavior of (4.1). Clearly, the asymptotic energy dependence is E^{-1} as for the OBK. The eikonal cross section is, however, reduced with respect to the OBK value by a significant factor. Asymptotically, when $\gamma\to\infty$, $\delta\to 1$, $\eta\to\alpha=\frac{1}{137}$, $p_-\to -1/\alpha$, the prefactor in (4.1), specific to the eikonal approximation, takes the form $[\pi\alpha Z_T/\sinh(\pi\alpha Z_T)]$ $\times\exp[-2\alpha Z_T\tan^{-1}(1/\alpha Z_T)]$ which ranges from 0.80 for $Z_T=10$, 0.33 for $Z_T=50$, to 0.15 for $Z_T=90$. Moreover, the last term in parentheses in (4.1) contributes another reduction factor whose size depends on both Z_P and Z_T. The combined effect of these factors is to diminish the eikonal cross section by a factor of 5–15 below the OBK value.[10]

V. EXTENSION TO ARBITRARY INITIAL AND FINAL STATES

The method outlined in Sec. III for $1s$-$1s$ capture can be readily generalized to arbitrary initial and final states. Adopting the usual relativistic notation[24] one may write a hydrogenic wave function as

$$\phi_{\kappa\mu}(\mathbf{r})=\begin{bmatrix} g_\kappa(r)\chi_\kappa^\mu(\hat{\mathbf{r}}) \\ if_\kappa(r)\chi_\kappa^\mu(\hat{\mathbf{r}}) \end{bmatrix}, \tag{5.1}$$

where χ_κ^μ is the well-known spin-angular function obeying the relation

$$(\boldsymbol{\sigma}\cdot\hat{\mathbf{r}})\chi_\kappa^\mu=-\chi_{-\kappa}^\mu . \tag{5.2}$$

With the aid of (5.2) it is convenient to express the spin-angular function with the higher orbital angular momentum by that of the lower one. For example, if $\kappa=-1$ (-2), corresponding to a large component with $s_{1/2}$ $(p_{3/2})$, one may rewrite the small component in (5.1) associated with $p_{1/2}$ $(d_{3/2})$ by using (5.2). If, on the other hand, $\kappa=1$, corresponding to a large component with $p_{1/2}$, it is advantageous to express the large component by $(\boldsymbol{\sigma}\cdot\hat{\mathbf{r}})$ acting on the small $(s_{1/2})$ component. For definiteness, when calculating P_h we assume that $\kappa<0$ so that $(\boldsymbol{\sigma}\cdot\hat{\mathbf{r}})$ appears with the small component as in Sec. III.

We first calculate the density matrix P_g of (2.16) by introducing the expansion (3.4) into the definition of g so that

$$g_{\kappa\mu}(\mathbf{q})=\left[\frac{2}{\pi}\right]^{1/2}\begin{bmatrix} a_\kappa\chi_\kappa^\mu(\hat{\mathbf{q}}) \\ b_\kappa(\boldsymbol{\sigma}\cdot\hat{\mathbf{q}})\chi_\kappa^\mu(\hat{\mathbf{q}}) \end{bmatrix} \tag{5.3}$$

with

$$a_\kappa=i^{l_\kappa}\int_0^\infty g_\kappa(r)j_{l_\kappa}(qr)r\,dr , \tag{5.4a}$$

$$b_\kappa=-i^{l_{-\kappa}+1}\int_0^\infty f_\kappa(r)j_{l_{-\kappa}}(qr)r\,dr . \tag{5.4b}$$

From (5.3) the density matrix $P_g^{\kappa\mu}$ can be directly derived, in analogy to (3.7). For an unpolarized ensemble we may, however, again take advantage of the powerful density-matrix formulation. With the aid of the readily verified property

$$\sum_\mu \chi_\kappa^\mu(\hat{\mathbf{q}})[\chi_\kappa^\mu(\hat{\mathbf{q}})]^\dagger=\frac{2j_\kappa+1}{8\pi}\begin{bmatrix}1&0\\0&1\end{bmatrix} \tag{5.5}$$

the unpolarized density matrix P_g is simply given by

$$P_g^\kappa=\frac{2j_\kappa+1}{4\pi^2}\begin{bmatrix} |a_\kappa|^2 & a_\kappa b_\kappa^*(\boldsymbol{\sigma}\cdot\hat{\mathbf{q}}) \\ a_\kappa^* b_\kappa(\boldsymbol{\sigma}\cdot\hat{\mathbf{q}}) & |b_\kappa|^2 \end{bmatrix} \tag{5.6}$$

which immediately reduces to (3.8) for $\kappa=-1$.

In a similar fashion we derive the density matrix P_h^κ (where, of course, κ need not be the same) for the initial state by introducing the complex vector $\mathbf{k}_\lambda$ as in (3.9). We then can write

$$h_{\kappa\mu}(\mathbf{k}_\lambda)=\left[\frac{2}{\pi}\right]^{1/2}\begin{bmatrix} \bar{a}_\kappa\chi_\kappa^\mu(\hat{\mathbf{k}}_\lambda) \\ \bar{b}_\kappa(\boldsymbol{\sigma}\cdot\hat{\mathbf{k}}_\lambda)\chi_\kappa^\mu(\hat{\mathbf{k}}_\lambda) \end{bmatrix} \tag{5.7}$$

with

$$\bar{a}_\kappa(\lambda)=i^{l_\kappa}[\Gamma(i\nu)]^{-1}\int_0^\infty g_\kappa(r)j_{l_\kappa}(k_\lambda r)e^{-\lambda r}r^2\,dr \tag{5.8a}$$

and

$$\bar{b}_\kappa(\lambda)=-i^{(l_{-\kappa}+1)}[\Gamma(i\nu)]^{-1}\times\int_0^\infty f_\kappa(r)j_{l_{-\kappa}}(k_\lambda r)e^{-\lambda r}r^2 dr . \tag{5.8b}$$

In constructing P_h^κ from (5.7) we have to observe that the (complex) angles $\hat{\mathbf{k}}_\lambda, \hat{\mathbf{k}}_{\lambda'}$ are generally not the same and hence (5.5) is not applicable. Instead, the addition theorem for spherical harmonics yields[14] a Legendre polynomial P_{l_κ} for the difference angle between the two. As a result, we have for (2.17a)

$$P_h^\kappa=\frac{2j_\kappa+1}{4\pi^2}\int_0^\infty d\lambda\int_0^\infty d\lambda'\begin{bmatrix}\bar{a}_\kappa(\lambda)\bar{a}^*_\kappa(\lambda') & \bar{a}_\kappa(\lambda)(\boldsymbol{\sigma}\cdot\hat{\mathbf{k}}^*_{\lambda'})\bar{b}^*_\kappa(\lambda')\\ \bar{b}_\kappa(\lambda)(\boldsymbol{\sigma}\cdot\hat{\mathbf{k}}_\lambda)\bar{a}^*_\kappa(\lambda') & \bar{b}_\kappa(\lambda)(\boldsymbol{\sigma}\cdot\hat{\mathbf{k}}_\lambda)(\boldsymbol{\sigma}\cdot\hat{\mathbf{k}}^*_{\lambda'})\bar{b}^*_\kappa(\lambda')\end{bmatrix}$$

$$\times\lambda^{i\nu-1}(\lambda')^{-i\nu-1}P_{l_\kappa}\left[\frac{1}{k_\lambda k^*_{\lambda'}}[p_b^2+p_-^2+ip_-(\lambda-\lambda')+\lambda\lambda']\right]. \tag{5.9}$$

In order for the λ and λ' integration to factor one has, in general, to expand P_l in a power series and then separate the terms in λ and λ'. For $l\leq 1$ the task is trivial, and cross-section formulas similar in structure to (3.17) and (3.18) can be worked out. The results are displayed in the Appendix for initial $2s_{1/2}$, $2p_{1/2}$, and $2p_{3/2}$ states and have previously been evaluated numerically in Ref. 10. For arbitrary combinations of κ_i and κ_f one has to work out (5.6) and (5.9) and insert the results into (2.18).

As in Sec. III the OBK approximation is easily derived as a special case. While P_g^κ of (5.6) remains unchanged, P_h^κ assumes the same structure as P_g^κ, except for the replacement $\mathbf{q}\rightarrow\mathbf{p}$, $Z_P\rightarrow Z_T$, and in the calculation of a,b the integrands in (5.4) which include the $1/r$ of the Coulomb potential have to be multiplied by r.

VI. RESULTS AND DISCUSSION

In the present work we have developed the eikonal theory for electron capture by relativistic projectiles. This approach is applicable if the kinetic energy of an electron traveling with the speed of the projectile is much greater than the binding energy in both target and projectile, or specifically for $1s$-$1s$ capture, if $\gamma-1\gg 1-(1-\alpha^2Z^2)^{1/2}$ where Z is the larger of the nuclear charges. As in the nonrelativistic version,[15,16] the prior form adopted here[27] (and appropriate for $Z_T\gtrsim Z_P$) includes multiple-scattering effects between the electron and target nucleus. However, it does not involve the small portion of phase space associated with hard-hard collisions that are responsible for the Thomas peak in the differential cross section. The asymptotic energy dependence E^{-1} is the same as for the first[3-5] or second[7] Born approximation.

The exact eikonal cross section can be expressed as a double integral (as compared to a one-dimensional integral for the OBK approximation[5]) which can be easily evaluated numerically for any explicitly given combination of initial and final states. In deriving the capture cross section for experiments that do not detect the electron spin polarization we have shown how the use of a density-matrix formalism significantly simplifies the calculations. This technique is, of course, equally advantageous if used with any other capture theory.

Since $1s$-$1s$ capture is the simplest and most important case, we have derived an approximate closed-form expression for the cross section in this case. The approximate formula is very accurate for small and intermediate charges[10] and only for the highest charges may be off by 40—50%. Figure 1 displays calculated capture cross sections for bare Ne nuclei impinging on one-electron targets with various nuclear charges. It is clearly seen from the figure that in the extreme relativistic limit the cross-section curves begin to fall off more slowly (as E^{-1}) than in the nonrelativistic theory (as E^{-6} or $E^{-11/2}$). The approximate expression (4.1) also allows one to distinguish contributions that arise from the interaction of the relativistically induced magnetic field of the projectile with the electron magnetic moment from contributions due to relativistic modifications of the initial and final electron orbits.

From both the exact and the approximate eikonal result, we can easily recover the corresponding OBK result.

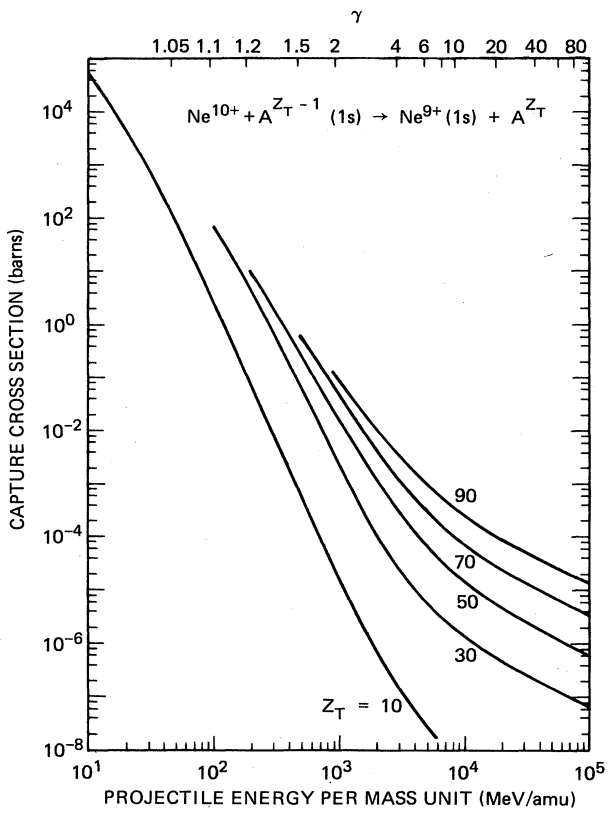

FIG. 1. Cross section for electron capture from a hydrogenic Dirac $1s_{1/2}$ orbital of the target with nuclear charge Z_T into a hydrogenic Dirac $1s_{1/2}$ orbital of a projectile with nuclear charge $Z_P=10$ is plotted as a function of the collision energy per nucleon. Cross sections are given in barns (10^{-24} cm^2). On the upper edge of the figure the projectile velocity v is expressed in terms of the relativistic parameter $\gamma=(1-v^2/c^2)^{-1/2}$. Cross-section curves are calculated according to Eq. (4.1). Each curve starts at projectile velocities that are about twice the K-shell electron velocity in the target.

In order to do so we just have to switch off the final-state interaction by setting $Z_T'=0$. While in the eikonal approach, for a one-electron system $Z_T'=Z_T$, it is tempting to use Z_T' as an *effective* final-state charge for a multielectron target. However, in the absence of a detailed theory for the final-state interaction, such a procedure should probably better not be applied.

A comparison with the OBK approximation shows that the eikonal cross section is significantly (by a factor of 5—15) smaller than the OBK and still much smaller than the second-Born-approximation result. In fact, it has been shown in Ref. 10 that this reduction is just what is needed to bring calculated cross sections into rather good agreement with experimental data for a number of collision systems and energies.

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APPENDIX: CAPTURE FROM INITIAL L-SHELL STATES

1. $2s_{1/2}$-$1s_{1/2}$ transitions

Electron capture from initial $2s_{1/2}$ states is completely analogous to capture from $1s_{1/2}$ states, except that the radial wave functions, and hence the integrals A_0,B_m defined in (3.10) and (3.11) have to be modified. Using the notation $s=(1-\alpha^2Z_T^2)^{1/2}$, $W=[\frac{1}{2}(1+s)]^{1/2}$, and $\zeta=Z_T/(2W)$ we can write the radial wave functions[24] as

$$g(r)=N_g r^{s-1}e^{-\zeta r}(c_0+c_1 r)\ ,$$
$$f(r)=N_f r^{s-1}e^{-\zeta r}(a_0+a_1 r) \tag{A1}$$

with

$$N_g=\frac{(2Z_T)^{s+1/2}}{2(2W)^{s+1}}\left[\frac{2s+1}{\Gamma(2s+1)(2W+1)}\right]^{1/2}(1+W)^{1/2}\ ,$$
$$N_f=-N_g\left[\frac{1-W}{1+W}\right]^{1/2}\ , \tag{A2}$$

and

$$c_0=2W,\quad c_1=-\frac{Z(2W+1)}{W(2s+1)}\ ,$$
$$a_0=2(W+1),\quad a_1=c_1\ . \tag{A3}$$

With the abbreviation $\lambda_\pm=\lambda+\zeta\pm ik_\lambda$ where k_λ is given by (3.9) we get the integrals

$$A_0(\mathbf{p})=\frac{N_g}{\Gamma(i\nu)}\left[c_0\Gamma(s+1)\int_0^\infty\frac{1}{2ik_\lambda}(\lambda_-^{-(s+1)}-\lambda_+^{-(s+1)})\lambda^{i\nu-1}d\lambda+c_1\Gamma(s+2)\int_0^\infty\frac{1}{2ik_\lambda}(\lambda_-^{-(s+2)}-\lambda_+^{-(s+2)})\lambda^{i\nu-1}d\lambda\right], \tag{A4}$$

$$\begin{aligned}B_m(\mathbf{p})=\frac{N_f}{\Gamma(i\nu)}\Bigg[&a_0\Gamma(s)\int_0^\infty\frac{1}{2ik_\lambda^3}(\lambda_-^{-s}-\lambda_+^{-s})\lambda^{i\nu-1+m}d\lambda-a_0\Gamma(s+1)\int_0^\infty\frac{1}{2k_\lambda^2}(\lambda_-^{-(s+1)}+\lambda_+^{-(s+1)})\lambda^{i\nu-1+m}d\lambda\\&+a_1\Gamma(s+1)\int_0^\infty\frac{1}{2ik_\lambda^3}(\lambda_-^{-(s+1)}-\lambda_+^{-(s+1)})\lambda^{i\nu-1+m}d\lambda\\&-a_1\Gamma(s+2)\int_0^\infty\frac{1}{2k_\lambda^2}(\lambda_-^{-(s+2)}+\lambda_+^{-(s+2)})\lambda^{i\nu-1+m}d\lambda\Bigg]\quad\text{with } m=0,1\ .\end{aligned} \tag{A5}$$

If these integrals are inserted into (3.18) we may use (3.17) for calculating the $2s_{1/2}$-$1s_{1/2}$ capture cross section for a single electron. Of course, the quantities $p_\pm$ defined in (2.15) have to be recalculated using the appropriate initial energies.

2. $2p_{1/2}$-$1s_{1/2}$ transitions

In this case, the large component of the initial state has a $p_{1/2}$ spin-angular function while the small component has $s_{1/2}$. It is hence advantageous in (5.1) to express χ_κ^μ by $\chi_{-\kappa}^\mu$ using (5.2). This means that $(\boldsymbol{\sigma}\cdot\hat{\mathbf{r}})$ appears in the large component and, consequently, the role of the A,B integrals is inverted, i.e., $A_0,B_m\rightarrow A_m,B_0$. Again using $s=(1-\alpha^2Z_T^2)^{1/2}$, $W=[\frac{1}{2}(1+s)]^{1/2}$, and $\zeta=Z_T/(2W)$ the radial wave functions[24] are given by (A1) but now with

$$N_g=\frac{(2Z_T)^{s+1/2}}{2(2W)^{s+1}}\left[\frac{2s+1}{\Gamma(2s+1)(2W-1)}\right]^{1/2}(1+W)^{1/2}\ ,$$
$$N_f=-N_g\left[\frac{1-W}{1+W}\right]^{1/2} \tag{A6}$$

and

$$c_0=2(W-1),\quad c_1=-\frac{Z_T(2W-1)}{W(2s+1)}\ ,$$
$$a_0=2W,\quad a_1=c_1\ . \tag{A7}$$

Owing to the formal interchange of large and small components as compared to the $2s_{1/2}$ case, the integrals are easily obtained by the following prescriptions: $A_m(\mathbf{p})$, $m=0,1$ is derived from $B_m(\mathbf{p})$ in (A5) by the replacements $N_f\to N_g$ and $a_0,a_1\to c_0,c_1$. Similarly, B_0 is derived from A_0 in (A4) by the substitution $N_g\to -N_f$ and $c_0,c_1\to a_0,a_1$. However, Q has now to be redefined as

$$\begin{aligned}Q=&m_{11}[\,|A_0|^2(p_b^2+p_-^2)+2\,\mathrm{Im}(A_0A_1^*)p_-+|A_1|^2]\\&+(2m_{12}/q)[\mathrm{Re}(A_0B_0^*)(p_b^2+p_+p_-)-\mathrm{Im}(A_1B_0^*)p_+]\\&+2m'_{12}[\mathrm{Re}(A_0B_0^*)p_--\mathrm{Im}(A_1B_0^*)]+m_{22}|B_0|^2\ .\end{aligned} \tag{A8}$$

When (A8) is inserted into (3.17) we obtain the $2p_{1/2}$-$1s_{1/2}$ capture cross section for a single unpolarized electron.

3. $2p_{3/2}$-$1s_{1/2}$ transitions

Since $\kappa<0$ in this case, the procedure is similar as for the $s_{1/2}$ initial state and is outlined in Sec. V. The result for the unpolarized density matrix P_h is given in (5.9) with $P_l(x)=P_1(x)=x$. With the definitions $s=(4-\alpha^2Z_T^2)^{1/2}$ and $W=s/2$ we have the normalization constants[24]

$$N_g=\frac{Z_T^{s+1/2}}{[2\Gamma(2s+1)]^{1/2}}(1+W)^{1/2}\ ,$$
$$N_f=-N_g\left[\frac{1-W}{1+W}\right]^{1/2}\ . \tag{A9}$$

In terms of $\lambda_\pm=\lambda+Z_T/2\pm ik_\lambda$ we get the λ integrals

$$A_m(\mathbf{p})=\frac{N_g}{\Gamma(i\nu)}\left[\Gamma(s)\int_0^\infty\frac{1}{2ik_\lambda^3}(\lambda_-^{-s}-\lambda_+^{-s})\lambda^{i\nu-1+m}d\lambda-\Gamma(s+1)\int_0^\infty\frac{1}{2k_\lambda^2}(\lambda_-^{-(s+1)}+\lambda_+^{-(s+1)})\lambda^{i\nu-1+m}d\lambda\right],$$
$$m=0,1 \tag{A10}$$

$$\begin{aligned}B_m(\mathbf{p})=\frac{N_f}{\Gamma(i\nu)}\Bigg[&3\Gamma(s-1)\int_0^\infty\frac{1}{2ik_\lambda^5}(\lambda_-^{-(s-1)}-\lambda_+^{-(s-1)})\lambda^{i\nu-1+m}d\lambda-\Gamma(s+1)\int_0^\infty\frac{1}{2ik_\lambda^3}(\lambda_-^{-(s+1)}-\lambda_+^{-(s+1)})\lambda^{i\nu-1+m}d\lambda\\&-3\Gamma(s)\int_0^\infty\frac{1}{2k_\lambda^4}(\lambda_-^{-s}+\lambda_+^{-s})\lambda^{i\nu-1+m}d\lambda\Bigg],\quad m=0,1,2\ .\end{aligned} \tag{A11}$$

Evaluation of the trace in (2.18) then yields [with $q=(p_b^2+p_+^2)^{1/2}$] the integrand to be used in (3.17) as

$$\begin{aligned}Q=&m_{11}[\,|A_0|^2(p_b^2+p_-^2)+2\,\mathrm{Im}(A_0A_1^*)p_-+|A_1|^2]\\&+(2m_{12}/q)[\mathrm{Re}(B_0A_0^*)(p_b^2+p_+p_-)(p_b^2+p_-^2)-\mathrm{Im}(B_1A_0^*)(p_b^2p_++p_b^2p_-+2p_+p_-^2)\\&\quad-\mathrm{Re}(B_2A_0^*)p_+p_-+\mathrm{Im}(B_0A_1^*)(p_b^2+p_+p_-)p_-+\mathrm{Re}(B_1A_1^*)(p_b^2+2p_+p_-)-\mathrm{Im}(B_2A_1^*)p_+]\\&+2m'_{12}[\mathrm{Re}(B_0A_0^*)(p_b^2+p_-^2)p_--\mathrm{Im}(B_1A_0^*)(p_b^2+2p_-^2)\\&\quad-\mathrm{Re}(B_2A_0^*)p_-+\mathrm{Im}(B_0A_1^*)p_-^2+2\,\mathrm{Re}(B_1A_1^*)p_--\mathrm{Im}(B_2A_1^*)]\\&+m_{22}[\,|B_0|^2(p_b^2+p_-^2)^2+4\,\mathrm{Im}(B_0B_1^*)(p_b^2+p_-^2)p_-\\&\quad+2|B_1|^2(p_b^2+2p_-^2)-2\,\mathrm{Re}(B_0B_2^*)p_-^2+4\,\mathrm{Im}(B_1B_2^*)p_-+|B_2|^2]\ .\end{aligned} \tag{A12}$$

With this Q Eq. (3.17) yields the cross section per electron for $2p_{3/2}$-$1s_{1/2}$ capture assuming an average over initial angular momentum projections and a sum over final spin states.

The formulas given in this appendix have been used in Ref. 10 for evaluating the cross sections for L-shell capture.

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[27]The post version appropriate to $Z_P > Z_T$ is obtained from the prior form (2.18) of the cross section (see Ref. 14) by replacing $Z_P \leftrightarrow Z_T$, $Z_T' \rightarrow Z_P' = Z_P$ and by interchanging initial and final states *except* for the statistical factor $(2j+1)$.