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Eikonal calculations of electron capture by relativistic projectiles

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The eikonal theory of electron capture by relativistic projectiles has been formulated, and calculations are presented for 140- to 2100-MeV/amu C, Ne, and Ar projectiles incident on a series of target atoms between Al and U. The eikonal calculations are in good agreement with measurements at high relative velocities.

In the past several years, there has been considerable interest in electron capture at very high projectile energies. However, the theoretical discussion has focused on asymptotic nonrelativistic energies. Recently, a large body of data[1] on relativistic heavy-ion-atom collisions has been analyzed[2] to extract, among other information, nonradiative electron-capture cross sections for a variety of collisions. While relativistic capture theories[3–7] are just beginning to emerge, the analysis of electron capture by relativistic projectiles clearly shows that the relativistic Oppenheimer-Brinkman-Kramers (OBK) approximation overestimates the cross sections by factors of 6 or more, so that neither a reduction by the familiar factor of 0.295 based on, but not justified by, a specific second Born calculation[8] nor the inclusion of relativistic second Born terms[7] brings the calculated values close to the experimental data. In this work we present a comparison with experiment that is based on a parameter-free relativistic capture theory, the eikonal approximation, which includes multiple-scattering contributions to the cross sections.

For projectiles in the intermediate nonrelativistic velocity range, the eikonal approximation[9–13] has proven to give reliable estimates for summed[10] and state-to-state cross sections[11] in symmetric or near-symmetric collisions. It has furthermore been shown[12,13] that physically the prior version of the theory (to be adopted here) describes a hard collision of the electron with the projectile nucleus, followed by multiple soft collisions with the target nucleus.

In the present Rapid Communication, we give a brief outline of a relativistic generalization of the eikonal approach, and a comparison of the results with experimental data[1,2] and with theoretical OBK[5] and the second Born approximation[7] calculations. The details of the theoretical development are given in a separate publication.[14] Besides $1s$-$1s$ transitions, we also include capture from initial relativistic $2s_{1/2}$, $2p_{1/2}$, and $2p_{3/2}$ states into final $1s_{1/2}$ states of the projectile.

It is convenient to describe the collision in the impact-parameter (**b**) picture with the hydrogenic target (charge Z_T) at rest and the projectile (charge Z_P) moving with a velocity v along a straight-line trajectory. The transition amplitude in atomic units is then given in the covariant form by[3,5,6,14]

$$A_{fi}(\mathbf{b},v)=-i\int dt\, d^3r\,\langle S^{-1}\psi_{f'}(\mathbf{r}'_P,t')\rangle[-iS^{-1}\gamma_\mu A'_\mu(\mathbf{r}'_P,t')S]\psi_i(\mathbf{r}_T,t)\;, \tag{1}$$

where the primed (unprimed) quantities refer to the projectile P (target T) frame, $\langle\psi\rangle\equiv\bar{\psi}$, $\bar{\psi}=\psi^+\gamma_4$, the γ_μ are the Dirac gamma matrices,[15] and $\gamma_\mu A_\mu$ is the electromagnetic interaction. The matrix S that takes the spinor ψ from the target to the projectile frame via the relation $\psi'(\mathbf{r}',t')=S\psi(\mathbf{r},t)$ is given by[15]

$$S=[\tfrac{1}{2}(\gamma+1)]^{1/2}(1-\delta\alpha_z)\;, \tag{2}$$

where $\gamma=(1-v^2/c^2)^{-1/2}$, $\delta=(v/c)\gamma/(\gamma+1)$, and α_z is the component of the Dirac[15] matrix $\boldsymbol{\alpha}$ in the beam direction.

In the prior form of the eikonal theory, appropriate for $Z_T\gtrsim Z_P$, the initial and final wave functions in their respective frames are

$$\psi_i=\phi_i(\mathbf{r}_T)\exp(-iE_it)$$

and

$$\psi_{f'}=\phi'_f(\mathbf{r}_{P'})\exp(-iE_ft')\exp\left[-iZ'_T\int_t^\infty\frac{d\tau}{r_T}\right]\;, \tag{3}$$

where ϕ_i and ϕ'_f are relativistic target and projectile eigenfunctions and E_i and E_f the corresponding eigenenergies including the electron rest mass. The final-state wave function contains a phase distortion caused by the electron-target action integral taken from the time of capture to infinity. The associated target charge is denoted by Z'_T so that, by letting $Z'_T=0$ in Eq. (3), one may obviously retrieve the OBK.[5]

The cross section for specific initial and final spin projections is obtained by taking the absolute square of the amplitude in Eq. (1), and integrating over the impact-parameter plane. While Moiseiwitsch and co-workers[5,7] have separately calculated non-spin-flip ($m_j=\pm\frac{1}{2}\rightarrow\pm\frac{1}{2}$) and spin-flip ($\pm\frac{1}{2}\rightarrow\mp\frac{1}{2}$) transitions, we find it enormously simpler to sum (average) over the (currently unobservable) spin projections from the outset by using a density-matrix formalism.[14] As a result, we obtain the final cross sections[14] in a form that requires the numerical evaluation of two-dimensional integrals, as compared with the one-dimensional integrals occurring in the OBK approximation.[5] The evaluation of the cross section poses no basic problem, and has been done for initial relativistic target K and L shells, and final projectile K shells for various collisions.

If both the target and projectile charges are small, meaning that αZ_T and αZ_P are much less than unity, where $\alpha = \frac{1}{137}$ is the fine-structure constant, we may expand in powers of αZ, and only retain the lowest-order terms. In this way, we may derive[14] an approximate closed formula for the $1s_{1/2}$-$1s_{1/2}$ cross section per electron in atomic units

$$\sigma_{1s\text{-}1s}{eik} = \frac{2^7 \pi Z_P^5 Z_T^5 (\gamma+1)}{5(Z_T^2 + p_-^2)^5 v^2 \gamma^2} \frac{\pi \eta Z_T'}{\sinh(\pi \eta Z_T')} \exp[-2\eta Z_T' \tan^{-1}(-p_-/Z_T)]$$
$$\times \left[1 + \tfrac{5}{4}\eta \frac{Z_T'}{Z_T} p_- + \tfrac{5}{12}\eta^2 \frac{Z_T'^2}{Z_T^2} p_-^2 + \tfrac{1}{6}\eta^2 Z_T'^2 - \delta^2 + \tfrac{5}{16}\delta^4 + \frac{5\pi}{18}\delta\alpha(Z_P + Z_T) \right.$$
$$- \frac{5\pi}{36}\delta^3\alpha(Z_P+Z_T) + \tfrac{5}{8}\delta^2 \frac{\gamma}{\gamma+1}\frac{Z_T'}{Z_T} + \tfrac{1}{4}\delta^2\eta^2 Z_T'^2 + \tfrac{5}{48}\delta^4\eta^2 Z_T'^2 - \tfrac{5}{8}\delta\alpha Z_T \eta Z_T'(1 - \tfrac{1}{2}\delta^2)$$
$$\left. - \frac{5\pi}{18}\delta\frac{\gamma}{\gamma+1}\alpha Z_P \frac{Z_T'}{Z_T} + \frac{5\pi}{28}\delta\left(\frac{\gamma}{\gamma+1}\right)^2 \alpha Z_P \frac{Z_T'^2}{Z_T^2} - \frac{5\pi}{28}\frac{\delta\gamma}{\gamma+1}\alpha(Z_P + Z_T - \delta^2 Z_P)\frac{Z_T'}{Z_T} \right], \quad (4)$$

where $\eta = 1/v$ and $p_- = \eta(E_f/\gamma - E_i)$. In the nonrelativistic limit, $\delta \to 0$, Eq. (4) collapses to the nonrelativistic eikonal cross section.[10]

Table I compares relativistic OBK calculations, eikonal calculations using Eq. (4), and numerical eikonal calculations of electron capture into the K shell of 1050-MeV/amu Ne ions. If we set Z_T' equal to zero in Eq. (4), we recover the OBK results of Ref. 5 [Eqs. (17) and (18)] to within about 6%. Column 4 of Table I gives the numerical evaluation of the exact eikonal cross sections with $Z_T' = 0$. Although the numerical evaluation and Eq. (4) agree at low αZ, the numerical cross sections are lower at large αZ, and are identical to those obtained by numerically evaluating the OBK [Eqs. (11)–(14) of Ref. 5].

Column 5 of Table I gives the numerical evaluation of the eikonal approximation with $Z_T' = Z_T$. The ratios of the eikonal cross sections (column 5) to the OBK calculations (column 4) are between 0.12 and 0.2, which is precisely what is needed to bring theory into better agreement with experiment. Note that calculations using Eq. (4) with $Z_T' = Z_T$ (column 7) are in good agreement with the numerical calculations with $Z_T' = Z_T$ (column 5) at low αZ, but are too high at large αZ, as was seen in the OBK calculations (columns 3 and 4).

For low Z_T and for the capture of outer-shell target electrons, the Dirac one-electron wave functions used in the numerical calculations are not appropriate, because the nuclear charge Z_T is partially shielded by inner-shell electrons in the neutral target atom. Traditionally, in calculations of inner-shell ionization,[16] shielding is incorporated by replacing the target atomic number by $Z^* = Z_T - \Delta Z$, where $\Delta Z = 0.3$ for the K shell and 4.15 for the L shell. For capture,[17] one sometimes uses $Z^* = (2n^2\epsilon)^{1/2}$, where ϵ is the electron binding energy and n is the principal quantum number.[2] Ultimately such recipes attempt to reproduce relevant properties of many-electron wave functions using one-electron wave functions having effective charges. For electron capture by relativistic projectiles, the high-momentum components in the target atomic wave functions at momentum $q \sim |p_-| \sim 50$–200 a.u. are most important. One measure of these components is the magnitude of the Compton profile $J(q)$ at large q, for which tabulations exist, based on Dirac Hartree-Fock wave functions.[18] We therefore calculated Compton profiles for the $1s$, $2s$, and $2p$ shells using Dirac wave functions, and found the values of Z^* that reproduce the Hartree-Fock Compton profiles. The resulting values of ΔZ are Z_T and q dependent, but we found that for $q > 50$ a.u., one can use $\Delta Z = 0.3$ for the K shell and 3 for the L shell, and reproduce the Compton profiles to within about 30% in all cases where K and L capture are significant in the present work ($Z_T > 13$ for K and $Z_T > 50$ for L). We believe that the use of these ΔZ values

TABLE I. Cross sections (in barns) for electron capture into the K shell of 1050-MeV/amu Ne ions. The numbered columns are described in the text. The number in parenthesis gives the power of ten multiplying the preceding number.

1 Z_T	2 OBK Reference 5	3 Eq. (4) $Z_{T'}=0$	4 Numerical $Z_{T'}=0$	5 Numerical $Z_{T'}=Z_T$	6 Ratio	7 Eq. (4) $Z_{T'}=Z_T$	8 Shielded K-K	9 Total K-$K+L$
13	3.9(−4)	4.1(−4)	4.1(−4)	0.81(−4)	0.20	0.80(−4)	0.71(−4)	0.73(−4)
30	2.3(−2)	2.4(−2)	2.4(−2)	0.37(−2)	0.15	0.37(−2)	0.33(−2)	0.36(−2)
47	0.179	0.175	0.173	0.0224	0.13	0.0227	0.0196	0.0222
73	0.84	0.82	0.68	0.083	0.12	0.099	0.070	0.090
92	1.34	1.26	0.84	0.114	0.14	0.170	0.095	0.144

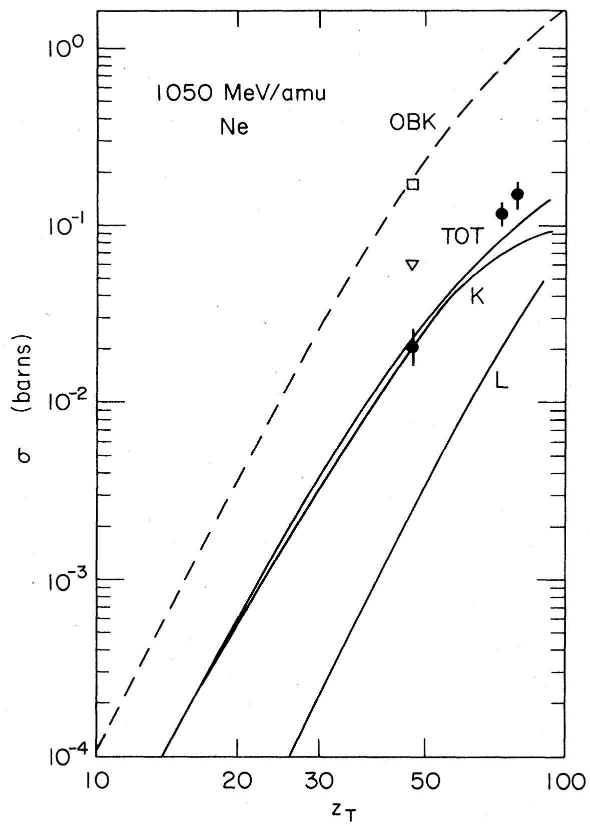

FIG. 1. Projectile K-electron-capture cross sections (per naked atom) for 1050-MeV/amu Ne ions. The OBK results (Ref. 5) are shown by the dashed lines and the □ point (Ref. 7), and the eikonal calculations with shielding for target K, L, and the sum of K and L capture are shown by the solid lines. A second Born approximation calculation is shown by the ∇ point (Ref. 7). Data (●) from Crawford and co-workers (Ref. 1) and Anholt (Ref. 2).

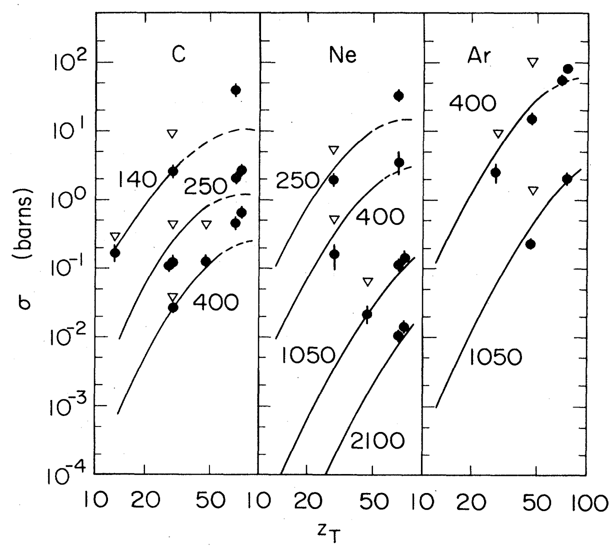

FIG. 2. Calculated eikonal projectile K-capture cross sections compared with measurements of Crawford and co-workers (Ref. 1) and Anholt (Ref. 2) and second Born calculations (Ref. 7) (∇ points, always lying immediately above the data points ●). The dashed part of the curves show the region where the eikonal approximation, including target K and L capture, may not be valid (see text).

should accurately account for many-electron effects on the target electron-capture cross sections to within about 30%.

Because zero-electron projectiles were used, unshielded Dirac projectile atomic wave functions are appropriate.

Column 8 of Table I gives the eikonal K-K–electron-capture cross sections including shielding, which are about 10%–20% lower than the Dirac cross sections in column 5. The effect of using a reduced charge for K-K transfer is seen at low $Z\alpha$. In column 8, we also used the experimental electron binding energies to calculate the momentum transfer. The difference between the shielded and unshielded cross sections at small αZ is due to using a smaller Z^* value, but at large αZ, it is due to the use of experimental binding energies. Finally, column 9 gives the total capture cross section into the K shell of the projectile from the $1s_{1/2}$, $2s_{1/2}$, $2p_{1/2}$, and $2p_{3/2}$ shells of the target atom.

Target L electron capture is significant at large Z_T, as shown in Fig. 1. For 1050-MeV/amu Ne ions, the eikonal results agree reasonably well with experiment. The OBK K-K transfer cross sections are factors of 5–10 too high, and a second Born calculation by Humphries and Moiseiwitsch[7] is a factor of 3 too high.

Figure 2 shows projectile K-capture sections for 140–2100-MeV/amu C, Ne, and Ar projectiles, compared with second Born calculations of K-K electron transfer and eikonal calculations including K and L target electron capture. It should be emphasized that the eikonal approximation is a high-energy approximation, which should be valid if the ion velocity v in atomic units is much greater than Z_P or Z_T, whichever is larger. The solid curves in Fig. 2 indicate where v is greater than $2Z_T$; the dashed lines show where v is less than $2Z_T$. For high velocities, the eikonal theory and experiment agree reasonably well, but for low velocities, the measured cross sections are higher than theory. Including M and N shell target electron capture should not affect the total calculated cross sections significantly. The second Born calculations[7] are always higher than experiment or the eikonal cross sections.

In conclusion, the eikonal approximation for electron capture, extended to relativistic projectile velocities, gives reasonable agreement with cross sections for low-Z_P projectiles obtained by Crawford and co-workers[1] and Anholt,[2] and therefore demonstrates the importance of multiple-scattering contributions. The poor agreement at low relative projectile velocities suggests that coupled-channel calculations may be needed there.

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