

Eikonal theory of charge exchange between arbitrary hydrogenic states of target and projectile

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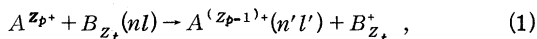
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The approach to electron capture previously developed by Chan and Eichler is extended to describe charge exchange in fast collisions between arbitrary hydrogenic states nl and $n'l'$ of target and projectile. A closed formula for the cross section is derived. As an illustration, cross sections for the reactions $H^+ + H(2l) \rightarrow H(3l) + H^+$ and $H^+ + H(n) \rightarrow H + H^+$ up to $n = 10$ are calculated. For the process $He^{2+} + H(n = 8,9) \rightarrow H^+ + He^+$, consistency with experimental results is obtained. Furthermore, a proposal is presented on how to apply the theory to multielectron targets by properly taking into account internal and external screening. As an example, Ar-L capture by protons is considered. Finally, the post and prior versions of the theory are compared and it is argued that the prior form currently used is more adequate for electron capture. A comparison between experimental and theoretical total cross sections for H(1s) electrons is briefly updated.

I. INTRODUCTION

In recent years much effort has been concentrated on the theory of electron capture into multicharged ions, both because of its basic interest and its importance for magnetically confined fusion plasmas. Most investigations¹⁻³ have been confined to capture from initial 1s states which are easiest to treat and most relevant for plasma processes. However, electron capture from higher initial states with principal quantum numbers $n \geq 2$ may also occur in fusion plasmas and, moreover, are important for multielectron targets and in the ionized regions of interstellar space.

In the present work we study the general process



where A denotes the projectile ion with charge Z_p and B the target atom with the effective charge Z_t determining the binding energy $\epsilon_t = -\frac{1}{2}Z_t^2/n^2$ (we use atomic units unless otherwise noted) and the wave function of the electron bound in the hydrogenic state nlm . We restrict ourselves to fast collisions, that is, to laboratory projectile velocities v greater than the orbital velocity of the electron involved or $E/M > 25 Z_t^2/n^2$ keV/amu.

The approach to be applied has been developed in previous publications²⁻⁴ and is based on the following three assumptions: (a) The projectile moves with a constant speed v on a rectilinear classical trajectory; (b) initial and final states are represented by travelling hydrogenic atomic orbitals; and (c) the final-state wave function is distorted by an eikonal phase factor. Thus, in the prior version of the theory, the electron-projectile interaction is treated in first order and the electron-target interaction in any order of perturbation theory, yet in the specific form given by the eikonal approximation. By taking into account the interaction of the captured elec-

tron with both the target and the projectile nucleus, one is led to a reduction of the cross section as compared to the Oppenheimer-Brinkman-Kramers (OBK) approximation by a factor of $\alpha = 0.15-0.4$ needed to bring theory²⁻⁴ in accord with experiment. It has been shown⁵ that the approach of Refs. 2-4 describes a close collision between electron and projectile followed by multiple distant collisions between electron and target nucleus. Because the distant collisions have a large weight in phase space this mechanism dominates capture at intermediate energies.

The cross section for electron exchange between arbitrary hydrogenic states has been given by Omidvar⁹ in the OBK approximation. Toshima¹⁰ has considered a few selected transitions between high-lying states in H atoms using the "full Born" approximation. The effect of internal and external screening in multielectron targets has been investigated by Nikolaev¹¹ in the OBK approximation.

In Sec. II the theory is presented in a fashion which is simpler in the notation than in Ref. 3 and is, of course, more general. The results are applied in Sec. III to the collision systems $H^+ + H(n)$, $He^2 + H(n)$, furthermore to multielectron targets by introducing a suitable treatment of screening effects and, finally, to derive the post version of the theory in order to compare it to the prior form. In Sec. IV a brief discussion of the present eikonal approach is given, and in Sec. V the results are summarized.

II. THEORY

It is convenient to formulate the charge exchange reaction (1) in the impact parameter picture from the outset thus ignoring terms of the order m/M (where m and M are electron and nuclear masses, respectively). In the laboratory frame, the projectile is assumed to move with a constant velocity v along the trajectory $\vec{R}(t) = \vec{b} + \vec{v}t$, where \vec{b} is the

impact parameter. The cross section, averaged over initial and summed over final magnetic sub-states, can be written as

$$\sigma_{nl-n'l'} = \frac{1}{2l+1} \sum_{m,m'} \int |A_{nlm-n'l'm'}(\vec{b}, v)|^2 d^2b. \quad (2)$$

In the prior version of the theory²⁻⁴ the transition amplitude is given by

$$A_{nlm-n'l'm'}(\vec{b}, v) = -i \int_{-\infty}^{\infty} \left\langle \Psi_{n'l'm'} \left| -\frac{Z_p}{r_p} \right| \Psi_{nlm} \right\rangle dt, \quad (3)$$

with

$$\Psi_{nlm} = \varphi_{nlm}(\vec{r}_t) e^{-i\epsilon_t t} e^{-i\vec{v}\cdot\vec{r}/2 - iv^2 t/8} \quad (4a)$$

and

$$\Psi_{n'l'm'} = \varphi_{n'l'm'}(\vec{r}_p) e^{-i\epsilon_p t} e^{i\vec{v}\cdot\vec{r}/2 - iv^2 t/8} \times \exp\left(-iZ'_t \int_t^{\infty} \frac{dt'}{r_t'}\right). \quad (4b)$$

Here, the vectors \vec{r} , $\vec{r}_t = \vec{r} + \frac{1}{2}\vec{R}$, and $\vec{r}_p = \vec{r} - \frac{1}{2}\vec{R}$ refer to the position of the electron with respect to the geometrical center, the target, and the projectile nucleus, respectively. Furthermore, φ_{nlm} and $\varphi_{n'l'm'}$ are hydrogenic wave functions and $\epsilon_t = -\frac{1}{2}Z_t^2/n^2$ and $\epsilon_p = -\frac{1}{2}Z_p^2/n'^2$ are the asymptotic eigenenergies in target and projectile. The velocity-dependent phase factors are recognized as the well known¹² translational factors and the last term in Eq. (4b) represents the eikonal phase factor. For later identification we here denote the effective target charge in the final state by Z'_t .

It is important to note that the time integral in the eikonal phase is evaluated for a *fixed position* \vec{r}_p of the electron with respect to the projectile. The eikonal phase thus describes the electron-target interaction integrated from the time of capture to infinity for an electron frozen in the projectile orbital. The integral actually diverges at the upper boundary; however, an infinitesimally small screening would remove this contribution without changing the cross section. In the following, we adopt the common practice of disregarding such contributions to the phase. In this connection, it should also be pointed out that if one were to include the nucleus-nucleus interaction as an operator in Eq. (3) this would enter into the correct choice of the boundary condition¹³ but would modify the transition amplitude only by a constant phase factor (again assuming an infinitesimal screening) and thus would not affect the cross section. An analysis of the amplitude (3) in terms of a perturbation expansion may be found in Ref. 5.

With Eqs. (2)–(4) we have set up the complete framework of the theory. There is no need to

introduce further approximations.

For the subsequent development it is now crucial to take advantage of the integral representation given by Gau and Macek¹⁴:

$$\exp\left(iZ'_t \int_t^{\infty} \frac{dt'}{r_t'}\right) = \exp[i\eta Z'_t \ln(r_t - z_t)] \\ = \frac{1}{\Gamma(-i\eta Z'_t)} \int_0^{\infty} \lambda^{-i\eta Z'_t - 1} e^{-\lambda(r_t - z_t)} d\lambda, \quad (5)$$

with $\eta = 1/v$. Moreover, we introduce the Fourier transforms h_{nlm} and $g_{n'l'm'}$ by the relations

$$\varphi_{nlm}(\vec{r}_t) e^{-\lambda(r_t - z_t)} = (2\pi)^{-3/2} \int h_{nlm}(\vec{p}; \lambda) e^{-i\vec{p}\cdot\vec{r}_t} d^3p \quad (6)$$

and

$$\varphi_{n'l'm'}(\vec{r}_p) \frac{1}{r_p} = (2\pi)^{-3/2} \int g_{n'l'm'}(\vec{q}) e^{-i\vec{q}\cdot\vec{r}_p} d^3q. \quad (7)$$

The function $g_{n'l'm'}$ is identical to the one defined in Ref. 3, but the general form of h_{nlm} was not needed there because only 1s initial states were considered. We now insert Eqs. (4)–(7) into Eq. (3) and evaluate the integrals $\int d^3r$ and $\int dt$. The former yields a three-dimensional delta function by which we can eliminate $\vec{q} = \vec{p} + \vec{v}$; the latter leads to the energy-conserving delta function which fixes the longitudinal components of $\vec{p} = (\vec{p}_b, p_z)$ and of $\vec{q} = (\vec{q}_b, q_z) = (\vec{p}_b, p_z + v)$ to be

$$p_z = \epsilon\eta - \frac{1}{2}v \quad (8a)$$

and

$$p_z = \epsilon\eta + \frac{1}{2}v, \quad (8b)$$

respectively, with $\epsilon = \epsilon_p - \epsilon_t$. It is then a simple matter to secure

$$A_{nlm-n'l'm'}(\vec{b}, v) = i \frac{2\pi\eta Z_p}{\Gamma(-i\eta Z'_t)} \int g_{n'l'm'}^*(\vec{p}_b, p_z) h_{nlm}(\vec{p}_b, p_z; \lambda) \\ \times \lambda^{-i\eta Z'_t - 1} e^{-i\vec{p}_b\cdot\vec{b}} d^2p_b d\lambda. \quad (9)$$

At this stage it is convenient to insert Eq. (9) into Eq. (2) and to evaluate $\int d^2b$. This at once gives us the cross section in the form

$$\sigma_{nl-n'l'} = \frac{1}{2l+1} \frac{(2\pi)^4 \eta^2 Z_p^2}{|\Gamma(-i\eta Z'_t)|^2} \\ \times \int G_{n'l'}(b_b^2 + p_b^2) H_{nl}(p_b^2 + p_z^2) d^2b, \quad (10)$$

where the quantities $G_{n'l'}(q^2)$ and $H_{nl}(p^2)$ have yet to be defined and calculated. We start with the quantity

$$G_{n'l'}(q^2) = \sum_m |g_{n'l'm'}(\vec{q})|^2, \quad (11)$$

which has already been calculated in Ref. 4. However, much simplification is achieved³ by summing over the subshells l' belonging to a given principal shell n' :

$$G_{n'}(q^2) = \sum_{l'=0}^{n'-1} G_{n'l'}(q^2) \\ = \frac{2q_n^3}{n^2(q^2 + q_n^2)^2}, \quad q_{n'} = Z_p/n'. \quad (12)$$

The summation in Eq. (12) has been performed by employing a sum rule—actually the addition theorem for four-dimensional spherical harmonics—originally given by Fock¹⁵ and later re-discovered by May¹⁶. In Eq. (11) it is convenient to factor out the simple expression for $G_{n'}$ given in Eq. (12) to obtain⁴

$$G_{n'l'}(q^2) = G_{n'}(q^2) \sum_{\lambda=l'}^{2n'-1} F_{\lambda}(n'l') \frac{q_n^{2\lambda}}{(q^2 + q_n^2)^{\lambda}}, \quad (13)$$

with

$$F_{\lambda}(n'l') = 2^{4l'}(2l'+1) \frac{(n'+l')!}{n'(n'-l'-1)!} \left(\frac{l'!}{(2l'+1)!} \right)^2 \\ \times \sum_{\substack{\mu=0 \\ \mu+\beta+\beta'+l'=\lambda}}^{l'} \sum_{\substack{\beta, \beta'=0 \\ \mu+\beta+\beta'+l'=\lambda}}^{n'-l'-1} (-1)^{\mu} \binom{l'}{\mu} B_{\beta}(n'l') B_{\beta'}(n'l'). \quad (14a)$$

Here, the coefficients

$$B_{\beta}(n'l') = \frac{(-n'+l'+1)_{\beta} (n'+l'+1)_{\beta}}{(l'+\frac{3}{2})_{\beta} \beta!} \quad (14b)$$

are expressed by the Pochhammer symbols $(a)_{\beta} = \Gamma(a+\beta)/\Gamma(a)$, $(a)_0 = 1$ and lend themselves to easy recursive computation

We now turn to the calculation of

$$H_{nl}(p^2) = \int_0^{\infty} d\lambda \int_0^{\infty} d\lambda' \sum_m [h_{nlm}(\vec{p}; \lambda) h_{nlm}^*(\vec{p}; \lambda')] \\ \times \lambda^{-in} Z_{l-1}(\lambda) (\lambda')^{in} Z_{l-1}(\lambda'). \quad (15)$$

This task is comparatively easy only for 1s initial states and in this case has implicitly been done in Refs. 3 and 4. In this work we derive the general form. If we decompose the initial electron wave function as $\varphi_{nlm}(\vec{r}) = R_{nl}(r) Y_{lm}(\hat{r})$ we may invert Eq. (6) to obtain

$$h_{nlm}(\vec{p}; \lambda) = (2\pi)^{-3/2} \int R_{nl}(r) Y_{lm}(\hat{r}) e^{-\lambda r} e^{i\vec{k}\cdot\vec{r}} d^3r \quad (16)$$

with the complex wave vector

$$\vec{k} = \vec{p} - i\lambda \hat{e}_z = (\vec{p}_{\perp}, p_z - i\lambda), \quad (17)$$

where \hat{e}_z is a real unit vector in the z direction. The set of angles associated with \vec{k} and denoted by \hat{k} includes a complex polar angle and an azimuth which is real and independent of λ . The analytic continuation of the spherical harmonics does not present any problems. We observe that in our case $Y_{lm}(\hat{k}) = (-1)^m Y_{l,-m}(\hat{k}^*)$. Introducing into Eq. (16) the expansion of the plane wave and integrating over the angles \hat{r} we obtain

$$h_{nlm}(\vec{p}; \lambda) = (2\pi)^{-3/2} 4\pi i^l \int R_{nl}(r) e^{-\lambda r} j_l(kr) r^2 dr Y_{lm}(\hat{k}), \quad (18)$$

where the argument of the spherical Bessel function $j_l(kr)$ is complex through the relation $k^2 = p_{\perp}^2 + p_z^2 - 2ip_z\lambda - \lambda^2$. The explicit form¹⁷ of the hydrogenic radial functions is now introduced and the radial integration¹⁸ is performed. Inserting into Eq. (15) and making use of the addition theorem for spherical harmonics, we obtain

$$H_{nl}(p_b^2 + p_z^2) = \frac{8(2l+1)q_n^{2l+3}}{n^2} \sum_{\beta, \beta'=0}^{n-l-1} \sum_{\nu=0}^{[\beta/2 + 1/2]} \sum_{\nu'=0}^{[\beta'/2 + 1/2]} (-1)^{\beta+\beta'} A_{\beta\nu}(nl) A_{\beta'\nu'}(nl) \\ \times \int_0^{\infty} d\lambda \int_0^{\infty} d\lambda' \lambda^{-in} Z_{l-1}(\lambda) (\lambda')^{in} Z_{l-1}(\lambda') \frac{\lambda_n^{\beta+1-2\nu} (\lambda')^{\beta'+1-2\nu'} k_{\lambda}^{l+2\nu} k_{\lambda'}^{*l+2\nu'}}{(\lambda_n^2 + k_{\lambda}^2)^{l+2+\beta} (\lambda_n'^2 + k_{\lambda'}^{*2})^{l+2+\beta'}} \\ \times P_l \left(\frac{1}{k_{\lambda} k_{\lambda'}^*} (p_b^2 + p_z^2 - ip_z(\lambda - \lambda') + \lambda\lambda') \right). \quad (19)$$

Here $[\frac{1}{2}\beta + \frac{1}{2}]$ denotes the integral part, $q_n = Z_p/n$, $\lambda_n = \lambda + q_n$, $k_{\lambda}^2 = p_b^2 + p_z^2 - 2ip_z\lambda - \lambda^2$, and P_l is a Legendre polynomial. Furthermore, from the initial wave function,

$$A_{\beta\nu}(nl) = n^{-1/2} [(n-l-1)!(n+l)!]^{1/2} (-[\frac{1}{2}\beta] - \frac{1}{2})_{\nu} 2^{2l+\beta+2\nu} q_n^{\beta} \frac{(l+1+\nu)!(2l+2+\beta)([\frac{1}{2}\beta + \frac{1}{2}]!)}{(2l+2+2\nu)!(n-l-1-\beta)!([\frac{1}{2}\beta + \frac{1}{2}] - \nu)! \beta! \nu!} \quad (20)$$

It is readily seen that k_λ and $k_{\lambda'}$ only enter in even powers and also that the expression (19) is manifestly real. The method of using complex angles in Eqs. (16) to (19) constitutes the basic device by which the treatment of arbitrary initial states has been achieved here.

In order to proceed further in the evaluation of $H_{n'l'}$, one has to expand P_l in a power series¹⁹ and then separate the various powers of λ and λ' occurring in Eq. (19). This involves several binomial and polynomial expansions and introduces a corresponding number of summations. At this expense, the integrations over λ and λ' are readily carried out.²⁰ Rather than presenting the result for $H_{n'l'}$ it is convenient to add the final small step from there to the calculation of the cross section. We have merely to insert $H_{n'l'}$ and Eq. (12) or (13) into Eq. (10). Noting that from the definitions (8a) and (8b)

$$p_b^2 + p_{\lambda'}^2 + q_n^2 = p_b^2 + p_{\lambda}^2 + q_n^2, \quad (21)$$

we can combine the denominators arising from $H_{n'l'}$ and $G_{n'l'}$, and perform $\int d^2 p_b = \pi \int dp_b^2$ to obtain the final result. The cross section (in atomic units) for the exchange of a single electron between the hydrogenic shells nl and $n'l'$ is given by

$$\sigma_{n'l-n'l'} = \frac{2^{8-l} \pi Z_i^5 Z_i^{5+2l}}{n^{5+2l} n'^3 v^2 (q_n^2 + p_{\lambda}^2)^{5+2l}} \frac{\pi \eta Z_i'}{\sinh(\pi \eta Z_i')} \exp[-2\eta Z_i' \tan^{-1}(-p_{\lambda}/q_n)] S(nl, n'l'), \quad (22a)$$

with

$$S(nl, n'l') = \sum_{\lambda=\lambda'}^{2n'-2} F_\lambda(n'l') q_n^{2\lambda} \sum_{\alpha, \alpha'} \sum_{\gamma=0}^{[l/2]} \sum_{\omega_1 \omega_2 \omega_3 \omega_4} \frac{(-1)^{\gamma(2l-2\gamma)!}}{(l-\gamma)!(l-2\gamma)!\gamma!} i^{\omega_3-\omega_2} (l-2\gamma; \omega_1 \omega_2 \omega_3 \omega_4) \\ \times \sum_{\rho=0}^{\omega_1+\sigma_1+\sigma_1'} (-1)^{\omega_1-\rho} (5+2l+\lambda+\beta+\beta'-s-s'-\rho)^{-1} \\ \times \binom{\omega_1+\sigma_1+\sigma_1'}{\rho} q_n^{2\omega_1-2\rho} p_{\lambda}^{2+\omega_3} (q_n^2 + p_{\lambda}^2)^{\rho-\beta-\beta'-\lambda} D_{\alpha\gamma} D_{\alpha'\gamma}^* \quad (22b)$$

and

$$D_{\alpha\gamma} = (-1)^{\sigma_1+\sigma_3+s} (-i)^{\sigma_2} 2^{2\sigma_2-s} A_{\beta\nu}(nl) (\gamma+\nu; \sigma_1 \sigma_2 \sigma_3) \binom{\beta+1-2\nu}{\tau} q_n^{\beta-2\nu-\tau+2\sigma_1} p_{\lambda}^{\sigma_2} (q_n + ip_{\lambda})^s \binom{s-1-i\eta Z_i'}{l+1+\beta}. \quad (22c)$$

In Eq. (22) the label α stands for a set of integers $\alpha = \{\beta \nu \sigma_1 \sigma_2 \sigma_3 \tau\}$ and correspondingly $\alpha' = \{\beta' \nu' \sigma_1' \sigma_2' \sigma_3' \tau'\}$. With the square brackets again denoting the integral part, the ranges of the summations are given by

$$\begin{aligned} \beta &= 0, 1, \dots, n-l-1, \\ \nu &= 0, 1, \dots, [\frac{1}{2}\beta + \frac{1}{2}], \\ \sigma_1, \sigma_2, \sigma_3 &= 0, 1, \dots, \gamma+\nu, \\ &\text{subject to } \sigma_1 + \sigma_2 + \sigma_3 = \gamma + \nu, \quad (23) \\ \tau &= 0, 1, \dots, \beta+1-2\nu, \\ \omega_1, \omega_2, \omega_3, \omega_4 &= 0, 1, \dots, l-2\gamma, \\ &\text{subject to } \omega_1 + \omega_2 + \omega_3 + \omega_4 = l-2\gamma. \end{aligned}$$

The parentheses $(k; k_1 k_2 \dots k_m) = k! / (k_1! k_2! \dots k_m!)$ polynomial coefficients,²¹ $s = \tau + \omega_2 + \omega_4 + \sigma_2 + 2\sigma_3$ and $s' = \tau' + \omega_3 + \omega_4 + \sigma_2' + 2\sigma_3'$. The binomial coefficient in Eq. (22c) is the usual finite product.

The quantity $F_\lambda(n'l')$ is given by Eq. (14). If, however, capture into a complete principal shell is to be calculated, it follows from Eq. (13) that $\sigma_{n'l-n'l'} = \sum_{l'} \sigma_{n'l-n'l'}$ is obtained by the simplifying replacement

$$F_\lambda(n'l') \rightarrow F_\lambda(n') = \delta_{\lambda 0}. \quad (24)$$

Within the eikonal theory Eq. (22) constitutes the universal cross-section formula for charge exchange between hydrogenic states. It is therefore not surprising that the result is quite complicated considering that already the corresponding OBK expression⁹ is rather involved. The OBK formula is obtained from Eq. (22) by putting $Z_i' = 0$. For hydrogen targets or if external screening can be disregarded one has $Z_i' = Z_i$. It should be noticed that for high velocities v the leading term in the cross section is proportional to $v^{-12-2l-2l'}$ as expected. For asymptotically high velocities the formula is, therefore, not

applicable.^{22,5}

For initial 2s states a compact formula for the cross section has already been published²³; for

$$\begin{aligned} \sigma_{2p \rightarrow n'} = & \frac{16\pi Z_t^5 Z_t'}{9n'^3 v^2 (q_n^2 + p_n^2)^6} \frac{\pi\eta Z_t'}{\sinh(\pi\eta Z_t')} \exp[-2\eta Z_t' \tan^{-1}(-p_n/q_n)] \\ & \times \left[1 - \frac{9}{10} \frac{Z_t'}{Z_t} + \frac{7}{32} \frac{Z_t'^2}{Z_t^2} + \left(\frac{93}{160} Z_t'^2 + \frac{1}{32} \frac{Z_t'^4}{Z_t^4} + \frac{9}{5} \frac{Z_t'}{Z_t} \epsilon - \frac{7}{8} \frac{Z_t'^2}{Z_t^2} \epsilon \right) \eta^2 \right. \\ & + \left. \left(\frac{1}{32} Z_t'^4 - \frac{1}{8} \frac{Z_t'^4}{Z_t^4} \epsilon + \frac{7}{8} \frac{Z_t'^2}{Z_t^2} \epsilon^2 \right) \eta^4 + \frac{1}{8} \frac{Z_t'^4}{Z_t^4} \epsilon^2 \eta^6 \right. \\ & \left. + \frac{1}{(q_n^2 + p_n^2)} \left[-\frac{3}{14} Z_t'^2 + \frac{2}{5} Z_t' Z_t' + \left(\frac{13}{56} Z_t'^2 Z_t'^2 - \frac{1}{20} Z_t' Z_t'^3 - \frac{4}{5} Z_t' Z_t' \epsilon \right) \eta^2 + \left(-\frac{1}{280} Z_t'^2 Z_t'^4 + \frac{1}{10} Z_t' Z_t'^3 \epsilon \right) \eta^4 \right] \right], \quad (25) \end{aligned}$$

with $q_n = Z_t/2$. For $Z_t' = 0$ and $n' = 2$ we recover the explicit result given by Omidvar.⁹

A computer program has been set up to calculate charge exchange cross sections from Eq. (22) for any given values of nl , $n'l'$, v , Z_t , Z_t' , Z_p , or summed cross sections. It is obvious that the computing time rapidly increases with increasing n .

It might be appropriate to give a brief summary of numerical checks to which Eq. (22) has been subjected: (a) Previous results^{3,4,23} for cross sections $1s \rightarrow n'$, $1s \rightarrow n'l'$, and $2s \rightarrow n'$ have been reproduced. (b) Independently computed results of Eq. (25) have been reproduced. (c) For $Z_t' = 0$ (in practice 10^{-8}) and given n and n' the numerical summation over l, l' reproduces the results of the elementary formula^{16,9,12} for $\sigma_{n \rightarrow n'}^{OBK}$. (d) For $Z_t' = 0$ the numerical calculations yield zero post-prior discrepancy¹² for the total capture cross section of 1s electrons. The prior version^{2,3} involves summations over many $n'l'$; the post version (see Sec. III D) involves summation over many n, l .

III. APPLICATIONS AND EXTENSIONS

A. Protons on excited hydrogen atoms

The general formula Eq. (22) of the preceding section, opens up a wide field of applications. The simplest capture reaction is provided by $H^+ + H(nl) \rightarrow H(n'l') + H^+$, where the cases of initial 1s and 2s states have been considered in previous publications^{2-4,23}. While capture from excited states of hydrogen certainly plays a role in plasma physics, there seems to be no relevant data available.

In Fig. 1 we present calculated cross sections [we use $Z_t = Z_t' = Z_p = 1$ in Eq. (22)] for all six possible transitions $2l \rightarrow 3l'$. It is seen from Fig. 1 that at low collision energies the cross sections increase with increasing l and l' , while at higher

convenience we give here the explicit result for capture from initial 2p states into a complete principal shell n' :

energies the cross sections increase with decreasing l and l' . This can be ascribed to the higher-momentum components prevailing in lower- l wave functions.¹⁷ The same qualitative behavior has been observed by Omidvar⁹ in his OBK calculations for the same system. It should be added that we find the same pattern also for higher values of n and n' .

For specific transitions between highly excited states (for example $4s-5p$, $5s-5p$, $8s-8s$, $8s-8p$) pronounced oscillations as a function of collision

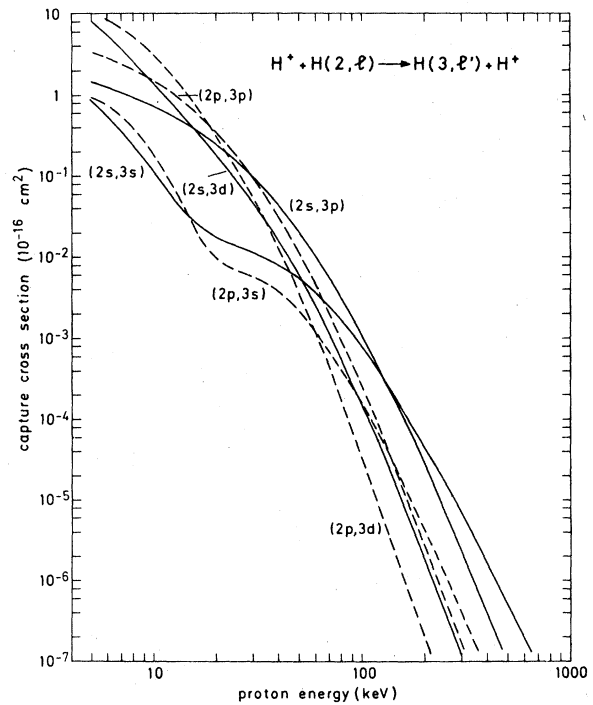


FIG. 1. Cross sections for charge exchange between the $n = 2$ and $n' = 3$ levels of hydrogen as a function of proton laboratory energy. Solid and dashed lines indicate initial 2s and 2p states, respectively.

energy have been found by Toshima¹⁰ in the capture cross section calculated in his "full Born" approximation. These oscillations are attributed¹⁰ to the internuclear potential; however, within the impact parameter picture adopted here, such contributions would be unphysical (they can be removed by a phase transformation^{13,5}) because the trajectories of the massive nuclei are—to a good approximation—unaffected by the electronic motion. Within our approach we have not been able to find such oscillations.

It is of some interest to study the capture cross section as a function of the initial principal quantum number n . From the geometrical size, one might expect the cross section to increase as n^4 ; on the other hand, the high-momentum components of the wave function¹⁷ decrease with increasing n and l . In Fig. 2 we have plotted the averaged cross section

$$\sigma(n) = n^{-2} \sum_{n'} \sum_{l=0}^{n'-1} (2l+1) \sigma_{nl-n'} \quad (26)$$

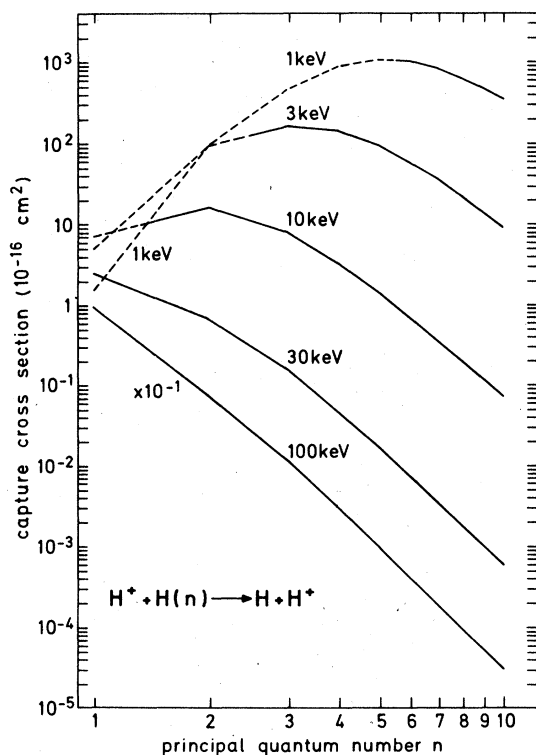


FIG. 2. Cross sections for charge exchange in the reaction $H^+ + H(n) \rightarrow H + H^+$ as a function of the initial principal quantum number n for various proton laboratory energies. The cross section is summed over all final shells n' . The solid and dashed straight lines connecting the points for integer n indicate collision velocities greater or smaller, respectively, than the Bohr orbital velocity of the electron in the target atom.

as a function of $\log_{10} n$ for various collision energies. It should be kept in mind that the eikonal theory can be expected to be applicable only if the collision velocity exceeds the relevant electronic orbital velocity, or if $E > 25/n^2$ keV. Those parts of the curves for which this requirement is met are drawn as solid lines. In the calculations the summation over the final principal shells has in most cases been extended up to $n' = 20$. Only for the higher energies $n' \leq 15$ is sufficient and also the highest values of l can be omitted from the calculation. At high values of n , computations based on Eq. (22) become uneconomical and it will be necessary to develop suitable asymptotic approximations.

It is concluded from Fig. 2 that the geometrical size of the excited target atom is reflected in the cross section only at low collision energies and probably becomes the determining feature only in the energy regime where the molecular approach has to be taken for describing the reaction. Certainly, these high-lying orbitals are sensitive to perturbations, in particular in slow collisions. For high energies the slope of the curves in Fig. 2 approaches a constant value, indicating an asymptotic behavior as $\sigma(n) \sim n^{-5}$. (For $E = 100$ keV we have $\sigma \sim n^{-4.9}$.) This asymptotic power law immediately follows from Eq. (22a) considering that mainly $l = 0$ contributes.

B. Fully stripped helium ions on excited hydrogen atoms

For the nonsymmetric system ${}^3\text{He}^{2+} + H(n)$ a beautiful experimental investigation has been conducted by Burniaux *et al.*²⁴ who studied the charge transfer for relative energies between 0.25 and 478 eV and initial principal quantum numbers n between 8 and 24. The experimental method involves merged beams and a time-correlation analysis of the reaction products. Field ionization has been used to modify and specify the population of the excited states. The results have been presented²⁴ as cross sections $\sigma(n_1, n_2)$ averaged over all n with $n_1 \leq n \leq n_2$.

For the present purpose of a comparison between experimental and theoretical results, unfortunately, only few data points can be used. This is because, firstly, the energy has to be high enough to make the theory applicable and, secondly, the principal quantum number has to be low enough to make computations still feasible. In Table I we present the experimental cross sections $\sigma(8, 9)$ together with the averaged theoretical values $\sigma_{\text{theor}}(8, 9) = \frac{1}{2}[\sigma(8) + \sigma(9)]$, where the summation over final states in Eq. (26) has been performed up to $n' = 40$. This is in accor-

TABLE I. Theoretical and experimental (Ref. 24) cross sections $\sigma(n)$ for the reaction $\text{He}^{2+} + \text{H}(n) \rightarrow \text{H}^+ + \text{He}^+$ assuming a statistical distribution over the initial states and capture into all final He^+ states with $n' \leq 40$. The experimental values contain contributions from $\sigma(7)$. The condition $E > 25/n^2$ keV is satisfied only for the highest energy given.

E_{rel} eV	$\sigma_{\text{theor}}(8)$	$\sigma_{\text{theor}}(9)$ (10^{-12} cm 2)	$\sigma_{\text{theor}}(8,9)$	$\sigma_{\text{expt}}(8,9)$
100	3.54	3.11	3.32	5.7
260	2.86	2.45	2.66	5.3
478	1.30	1.02	1.16	≤ 2.2

dance with the measurements²⁴ in which $\text{He}^+(n')$ with $n' > 40$ cannot be detected because it is field-ionized in the magnetic analyzer. Considering experimental uncertainties and the fact²⁴ that actually the experimental cross section labeled $\sigma(8,9)$ contains some contribution from $n=7$ and hence is likely to be overestimated, the agreement between the simple theory and experiment is quite satisfactory. It would be desirable to compare with data over a wider range in energies and initial states.

C. Multielectron targets

While capture experiments involving well defined hydrogenic systems (see Sec. III B) are extremely difficult to perform and correspondingly scarce, there is a large body of data available²⁵ on electron capture from higher principal shells ($n \geq 2$) in multielectron targets. Of course, the theoretical treatment is then complicated by many-body effects. If, nevertheless, we want to adapt the single-electron picture described in Sec. II to this case we shall try to simulate the main features of Hartree-Fock single-electron states by adjusting the parameters available in our bare-nuclei (hydrogenic) approximation.

(a) *The interior part of the Hartree-Fock wave function* is reasonably well approximated by a hydrogenic wave function φ_{nlm} with an effective Z_t derived, for example, from Slater's rules (internal screening²⁶). It is just this part that gives rise to the high- and intermediate-momentum components in the initial momentum distribution which dominate electron capture.

(b) *The tail of the Hartree-Fock wave function*, on the other hand, determines the Hartree-Fock eigenenergy ϵ_t and hence the removal energy for the electron considered. This tail is subject to additional screening by the outer electrons (external screening²⁶). The modulus of the eigenvalue is, therefore, less than the hydrogenic value calculated from the effective charge Z_t . This fact can be expressed by introducing a parameter

$\theta \leq 1$ through the relation

$$\epsilon_t = \theta^{\frac{1}{2}} Z_t^2 / n^2. \quad (27)$$

It is noticed that in the calculation of the capture amplitude, Eq. (3), ϵ_t enters in the energy-conserving delta function arising from the time integration. Obviously, one should use the correct ϵ_t (Hartree-Fock or experimental) at this point. Thus, in Eq. (4a) we make φ_{nlm} resemble the interior part of a Hartree-Fock wave function (by introducing the effective charge Z_t) and let ϵ_t be determined by the tail of the Hartree-Fock wave function (by adjusting θ to the electron removal energy). The resulting inconsistency is common¹¹ and unavoidable when using hydrogenic wave functions.

(c) As a third screening effect we have to consider that the *final-state interaction of the captured electron with the target nucleus* is increasingly shielded as the electron moves away from its original orbit. In order to account for this effect in a simple way, the effective eikonal charge Z'_t in Eq. (4b) should be chosen different from Z_t . In fact, if the original target was neutral, we have $Z'_t = 1$ once the captured electron has been carried outside the electron cloud of the target. Similarly, if capture occurs from an inner shell of a heavier target atom into the spatially more extended orbits of a lighter projectile ion, we expect that Z'_t should be considerably reduced from Z_t and may be close to 1. (Of course it would be desirable to have a more quantitative estimate for Z'_t .)

The approximations (a), (b), and (c) assign the quantities Z_t , θ , Z'_t , to three distinct screening effects: internal and external screening and the final-state interaction. While Z'_t appears explicitly in the final result one has to separate the effects of the momentum distribution (involving Z_t) from the effects of the energy conservation (involving θ) in the calculation. Clearly, the quantities p_+ and p_- defined in Eq. (8) have to be altered in accordance with Eq. (27). Then the only change of H_{nl} given in Eq. (19) is effected by substituting for p_+ the modified momenta

$$\tilde{p}_\pm = (\epsilon_p - \theta^{\frac{1}{2}} Z_t^2 / n^2) \eta \pm \frac{1}{2} v. \quad (28)$$

In Sec. II the final result, Eq. (22), is obtained by combining the energy denominators of $G_{n'l'}$, Eqs. (12) and (13), with those of H_{nl} because of relation (21). Yet this relation is valid only for Coulombic energies or $\theta = 1$. For $\theta < 1$ a rigorous treatment is also possible²⁷ [without taking recourse to Eq. (21)] but at the expense of considerable complications even for the lowest initial shells n . In order to avoid such complications and to keep the generality of the result, Eq. (22),

we may use Eq. (21) in the form

$$p_b^2 + \tilde{p}_+^2 + q_n^2 = p_b^2 + \tilde{p}_-^2 + \theta q_n^2 \quad (21')$$

and subsequently replace θq_n^2 by q_n^2 on the right-hand side. This replacement only affects terms arising from $G_{n'l}$, and allows us to combine them with similar terms originating from H_{nl} . The approximation thus introduced for mathematical convenience should be valid for those parts of the integral $\int d^2 p_b$ in which $p_b^2 \gg q_n^2$ and, generally, for $v^2 \gg q_n^2$. With this additional approximation, the capture cross section approximately including external screening effects may again be expressed by Eq. (22) yet with p_- formally replaced by \tilde{p}_- as defined in Eq. (28). Considering the simplicity of this result it should be worthwhile to test it against experiment in spite of deficiencies brought in by the approximation. In Fig. 3, as an example, we present a comparison between experimental²⁸ and theoretical results for the capture of Ar-L electrons by energetic protons. Since the L shell is fully occupied, the theoretical cross section is obtained as $\sigma_L = 2\sigma(2s) + 6\sigma(2p)$. The parameters used are $Z_t = 13.85$ according to the Slater rules and $Z'_t = 1$ according to the arguments given above. (If we would use $Z'_t = 2$ instead, the cross sections would be only very slightly reduced.) For comparison, three different values of θ have been used: $\theta = 1$ corresponds to the absence of external screening, $\theta = 0.412$ follows from the averaged L-shell binding ener-

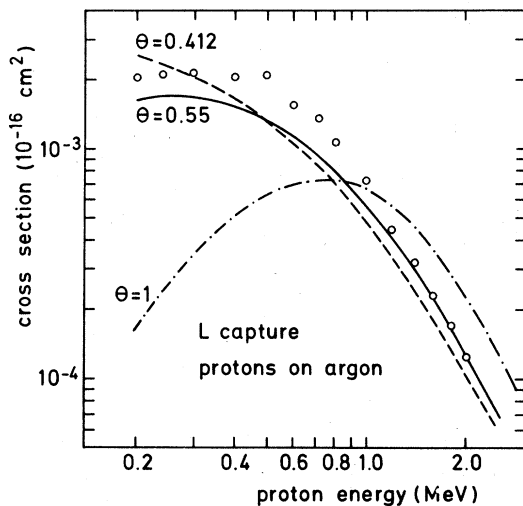


FIG. 3. Cross sections for capture of Ar-L electrons by protons as a function of proton laboratory energy. Experimental points are from Ref. 28. The theoretical cross sections are summed over all initial $2s$ and $2p$ states in argon using $Z_t = 13.85$, $Z'_t = 1$, $Z_p = 1$. Three different values have been used for the screening parameter θ . The proton velocity exceeds the electron orbital velocity at energies greater than 1.2 MeV.

gies,²⁹ and $\theta = 0.55$ gives a better fit to the experimental data. It should be noted here that the criterion $v > v_e$ for the validity of the eikonal theory requires proton energies $E > 25 Z_t^2/4$ keV ≈ 1200 keV and the additional approximation discussed above may require even higher energies. The lower portion of the energy scale is shown mainly to exhibit the great influence of binding-energy corrections for these energies. For higher energies the curves show little sensitivity to the choice of the binding energy.

D. Post version of the theory

As a final application, we consider a more theoretical problem. In the present work and before²⁻⁵ we have used the prior form of the eikonal theory, mainly for mathematical convenience. In fact, if the initial state is a $1s$ state,²⁻⁵ the Fourier transform Eq. (6) is easily performed and the aim of utilizing,^{2,3} Fock's sum rule¹⁵ forces us to combine the *final-state* wave function with the Coulomb potential in Eq. (7). Starting from the general formulation given in the present work, both the prior and the post version can be calculated on equal footing. Clearly, for the rigorous solution of the problem both versions agree but, as is obvious from the first-order Born approximation,¹² agreement is by no means a sufficient criterion for the reliability of an approach. Nevertheless, it is interesting and necessary to compare the two results. There are few theories for which this has actually been done.

In the post version of the theory one has to replace the transition amplitude, Eq. (3), by

$$A_{nlm-n'l'm'}^{\text{post}}(\vec{b}, v) = -i \int_{-\infty}^{\infty} \langle \Psi_{n'l'm'} | -\frac{Z_t}{r_t} | \Psi_{nlm} \rangle dt, \quad (29)$$

where now the eikonal phase factor is associated with the initial state

$$\begin{aligned} \Psi_{nlm} = \varphi_{nlm}(\vec{r}_t) e^{-i\epsilon_t t} e^{-i\vec{v} \cdot \vec{r}_t / 2 - i v^2 t / 8} \\ \times \exp\left(i Z'_p \int_{-\infty}^t \frac{dt'}{r_p}\right), \end{aligned} \quad (30a)$$

and

$$\Psi_{n'l'm'} = \varphi_{n'l'm'}(\vec{r}_p) e^{-i\epsilon_p t} e^{i\vec{v} \cdot \vec{r}_p / 2 - i v^2 t / 8}. \quad (30b)$$

Here, the effective projectile charge in the initial state has been denoted by Z'_p . The time integral in the eikonal phase is evaluated for a *fixed position* \vec{r}_t of the electron with respect to the target nucleus.³⁰ The eikonal phase thus describes the interaction prior to capture of the projectile with the electron frozen in the initial target orbital.

By inserting Eqs. (30) into Eq. (29) and follow-

ing the procedure outlined in Sec. II we obtain the transition amplitude in the form

$$A_{nlm \rightarrow n'l'm'}^{\text{post}}(\mathbf{b}, v) = i(-1)^{m+m'} \frac{2\pi\eta Z_t}{\Gamma(-i\eta Z_t')} \times \int g_{nl, -m}^*(\vec{p}_b, -p_-) h_{n'l', -m'}(\vec{p}_b, -p_+; \lambda) \times \lambda^{-inZ_t'^{-1}} e^{i\vec{p}_b \cdot \vec{b}} d^2 p_b d\lambda. \quad (31)$$

This expression has to be compared with the prior amplitude Eq. (9). When inserting into Eq. (2) it is immediately seen that the post form of the cross section is obtained from the prior form by the simple replacements $Z_p \rightarrow Z_t$, $Z_t' \rightarrow Z_p'$, and $nl \rightarrow n'l'$, so that

$$\sigma_{nl \rightarrow n'l'}^{\text{post}}(Z_p, Z_p', Z_t'; v) = \sigma_{n'l' \rightarrow nl}^{\text{prior}}(Z_t, Z_t', Z_p; v). \quad (32)$$

This is a generalization of the result previously derived⁵ for 1s-1s capture.

Equation (32) has been used in conjunction with Eq. (22) to compute the post version of the cross section for the reaction $\text{He}^{2+} + \text{H}(1s) \rightarrow \text{He}^+(n) + \text{H}^+$.

Figure 4 shows the calculated cross sections for both the prior and the post version for $n=1, 2$, and 3. The cross sections are divided by the corresponding OBK values (which are the same in both versions¹²) in order to provide a linear scale. In all three cases the post-prior discrepancy decreases with increasing energy. For 1s-1s transitions the discrepancy is about 15% or less for collision velocities twice or more than the orbital velocities in target and projectile.⁵ For $n \geq 2$ the relative discrepancies are substantially larger at low energies. For the total cross section the post curves are always lower than the prior curves. This tendency is increased

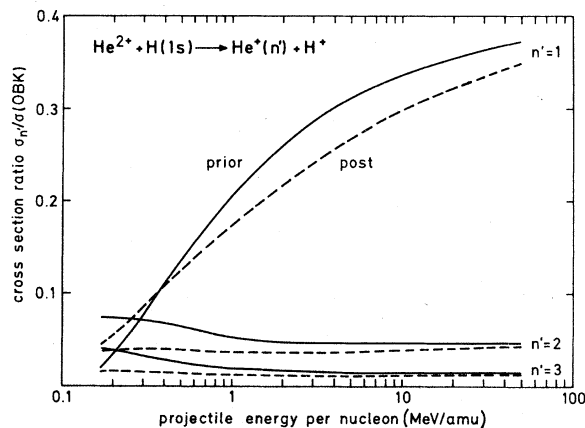


FIG. 4. The cross-section ratio $\sigma/\sigma^{\text{OBK}}$ for the reaction $\text{He}^{2+} + \text{H}(1s) \rightarrow \text{He}^+(n) + \text{H}^+$ as a function of the laboratory energy per nucleon. The solid and the dashed lines correspond to the prior and to the post form of the eikonal theory, respectively.

if He^{2+} is replaced by Li^{3+} . It, furthermore, turns out that experimental data points^{31,32} are usually between the curves but much closer to the prior curve.

This general behavior can be understood in the light of the discussion given in Ref. 5. It has been shown there that the prior form of the eikonal approximation describes a close collision of the electron with the projectile nucleus (associated with a large momentum transfer) followed by multiple distant collisions with the target nucleus (associated with smaller momentum transfers). Correspondingly, in the post version of the theory, we have multiple distant collisions of the electron with the projectile nucleus followed by a close collision with the target nucleus. Since it is physically obvious that a close collision between electron and projectile nucleus is instrumental for the capture process, *we expect that the prior and not the post version of the eikonal theory gives a more adequate description of electron capture.*

IV. FURTHER DISCUSSION OF THE EIKONAL APPROACH

In the preceding sections we have worked out and applied the classical trajectory eikonal method to the most general transitions between Coulombic states. Nevertheless, the simplest, and for practical purposes most important, transitions are those of the type 1s- n' investigated in Refs. 2 and 3. We have shown there that the ratio between the total cross section and the OBK cross section as a function of energy follows an almost universal curve (i.e., for all projectile and target charges). Since some new experimental data are now available for well defined one-electron systems it may be useful (see Fig. 5) to present a comparison between experimental³¹⁻³⁸ and theoretical^{2,3} total cross sections for *electron capture by bare projectiles from atomic hydrogen* (an exception is the cross sections for Fe^{20+} and Fe^{25+}). As is seen from Fig. 5 there is excellent agreement between theory and experiment for the lightest projectiles even at rather low projectile energies. With increasing projectile charge and for not too high energies (for $Z_p = 5, 6$), the theory seems to overestimate the cross sections, but again for $Z_p = 20, 25$ the agreement is surprisingly close. It should be remembered that the theoretical cross sections are given by a very simple formula^{2,3} which is applicable to high principal shells n' as well as to low ones. These contributions cannot easily be estimated otherwise be-

cause they vary as $(n')^{-3}$ only for high n' and at high energies.

With regard to scaling laws of the form

$$\sigma \sim Z_p^\alpha \quad (33)$$

for the total cross sections it has been shown by Day *et al.*³⁹ that α varies slowly with collision energy in the range of $\alpha = 3.0 \pm 0.12$. This is in good agreement³⁹ with experimental data^{37,40} and with the results of calculations⁴⁰ within the classical-trajectory Monte Carlo method^{1,6} yielding $\alpha = 2.9 \pm 0.1$ for $\text{Fe}^{Z_p^+} (Z_p = 10, 15, 20, 25) + \text{H}$ at 262 keV/amu.

In view of these encouraging features of the simple eikonal theory^{2,3} it may shed some light on the important ingredients of capture theories if we

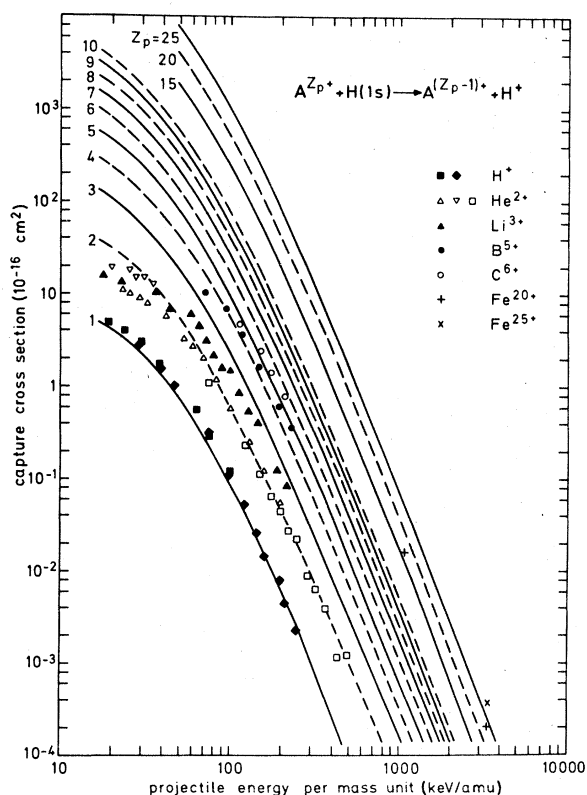


FIG. 5. Cross sections for the capture of $\text{H}(1s)$ electrons by bare projectiles with the charge Z_p , as a function of the laboratory energy per nucleon. The curves are calculated from the eikonal theory, Refs. 2 and 3. The points indicate experimental data. Solid symbols are associated with solid curves, open symbols with dashed curves. Solid squares and diamonds are from Refs. 34 and 35, respectively; open triangles, inverted triangles, and squares are from Refs. 31, 33, and 32, respectively; solid triangles are from Ref. 36; solid and open circles are from Ref. 37; the crosses are from Ref. 38. In all cases except the Fe data atomic hydrogen targets have been used.

briefly compare with the highly successful¹ unitarized distorted wave approximation (UDWA) proposed by Ryufuku and Watanabe.⁸ Both approaches have some aspects in common: they use classical rectilinear trajectories for the projectile, travelling atomic orbitals for the electrons, and they adopt some kind of sudden approximation by ignoring the time ordering of interactions. However, there are at least two basic differences. (a) The eikonal theory uses asymptotic (atomic) electron binding energies throughout the collision. On the other hand, the UDWA takes into account the time development of the diagonal part of the interaction; that is, the electron binding energies in the transient quasimolecule are treated in perturbation theory. As has been suggested by Ryufuku and Watanabe⁸ this seems to be the decisive reason why the UDWA works down to collision energies of 1 keV/amu and lower. We also may refer back to Fig. 3 to illustrate the importance of binding-energy corrections at low energies. (b) The eikonal theory treats the interactions of the electron to second and higher order (in some approximation), and particularly the second-order correction is instrumental^{4,5,22} in reducing the cross section by a factor of about 3 with respect to the OBK value at high energies. On the other hand, the UDWA ignores all non-diagonal matrix elements of the interaction except for those containing the initial state.⁸ This necessarily means that only *odd orders* in these matrix elements are included and, in particular, the second order is absent. This may largely explain the overestimation of the cross section⁸ by a factor of about 3; partially, it may also be due to the neglect of excitation and ionization channels among the intermediate states as has been pointed out in Ref. 8.

In short, it appears that for a more complete theory, binding-energy corrections are important at low collision energies and second-order (and higher-order) nondiagonal matrix element are important at higher energies.

V. SUMMARY AND CONCLUSIONS

In the present work the eikonal theory developed in earlier publications has been extended to charge exchange between arbitrary initial and final hydrogenic states nl and $n'l'$. Apparently, there is no other theory available beyond the OBK approximation that offers a systematic and closed-form solution for the charge exchange cross section. After sufficient experimental testing the result obtained may be of value in situations in which experimental information is not easily accessible. For example, the optical diagnostics of hot plasmas requires charge exchange cross sections as

input data. The final cross-section formula presented here can be readily evaluated for any set of parameters nl , $n'l'$, Z_p , Z_t , Z_t' , and v . Numerical computation times are very short for low values of n but rapidly increase with increasing n . For this limit, it would be desirable to develop a simplified asymptotic treatment.

An expression as general as Eq. (22) opens up a wide field of possible applications. As a first illustration, we have calculated the n dependence up to $n=10$ of the capture cross section in the reaction $H^+ + H(n) \rightarrow H + H^+$ for various collision energies, and also the subshell cross sections for all transitions in $H^+ + H(2l) \rightarrow H(3l') + H^+$. In the second example, $He^{2+} + H(n) \rightarrow H^+ + He^+$, experimental data²⁴ available for $n=8$ and $n=9$ confirm the calculated cross sections. Another field of application is provided by multielectron targets. Here a suitable choice has to be made for the parameters Z_t and θ describing inner and outer screening, respectively, and for the effective target charge Z_t' in the final state. A first comparison with experimental results²⁸ for Ar-L capture by protons shows encouraging agreement. The effect of projectile screening not considered here will be treated in a future publication⁴¹ for capture of 1s electrons.

The general formula Eq. (22) also serves as a starting point to compare the post and the prior form of the theory. It is argued that the prior version used currently and before²⁻⁵ should be

more appropriate for a description of electron capture.

In a final section, we update our earlier^{2,3} comparison between experimental and theoretical total cross sections for the capture of 1s electrons from atomic hydrogen into bare projectiles. From the overall and partly excellent agreement we draw confidence in estimating unknown cross sections for the applications mentioned above. The main shortcomings of the approach seem to occur at low collision energies and high charges Z_p . Arguments are given that this limitation arises from keeping the electron binding energies fixed at their asymptotic values throughout the collision. It is currently not clear how this point can be improved without completely destroying the simplicity of the theory.

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