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Eikonal calculation of electron-capture cross sections from an arbitrary *nlm* shell of a hydrogenic target into an arbitrary *n'l'm'* shell of a fast bare projectile

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Using techniques similar to those previously employed, we apply the eikonal approximation to the evaluation of the cross section for electron capture from an arbitrary *nlm* shell of a hydrogenic target atom into an arbitrary *n'l'm'* of a fast hydrogenic projectile. The results are obtained in exact analytical closed form. Numerical results are presented for the case $H^+ + H(1s) \to H(n'l'm') + H^+$ when $n' = 2$ and 3. Comparison is made with the corresponding Oppenheimer-Brinkman-Kramers (OBK) results.

I. INTRODUCTION

Charge-transfer processes have been of interest since the early days of quantum mechanics. This interest has increased considerably in the past few years, the focus being on processes relevant to magnetically confined-fusion plasmas and astrophysical plasmas. Knowledge concerning the charge transfer from a hydrogenic atom to a bare ion is important not only with regard to these applications but also from a fundamental point of view since such a process is the simplest type of a rearrangement reaction.

An approach for treating electron capture into arbitrary principle shells of energetic projectiles based on the eikonal approximation was developed by Chan and Eichler.[1] They later amended their approach for capture into arbitrary n', l' sublevels of a fast projectile from the ground state[2] as well as from an arbitrary initial n, l sublevel[3] of a hydrogenic target. The results obtained agree well with experimental findings for hydrogen and helium targets. In this paper we extend the eikonal treatment to cover n, l, m contributions. There are at least two reasons why such a study is interesting. First of all, specification of these contributions allow for a sterner test of capture theories. Such a test is realizable since techniques for measuring charge exchange for $p + N_2 \to N_2^+ + H(n' = 3, l', m')$ have recently been developed[4] and a corresponding study of charge capture for $p + H$ collisions is now underway at Harvard University.[5] The present study is partly motivated by these experimental interests. Secondly, it is the most general case and it contains all the previous results[1-3] as special cases. In addition, it furnishes information not available from classical trajectory Monte Carlo calculations.[6]

In Sec. II, we use the eikonal approximation to calculate the cross section for the capture of an electron into an (n', l', m') state of an energetic projectile from a hydrogenic target initially in the (n, l, m) state. The result is obtained in closed form, and is exact within the eikonal approximation. In Sec. III, we discuss our results and present some theoretical data for the reaction $H^+ + H(1s) \to H(n' = 2, 3, l', m') + H^+$. The Oppenheimer-Brinkman-Kramers (OBK) results are obtained as a limiting case and are given in the Appendix.

II. THEORY

We consider the process in which an electron, initially in the n, l, m state of a hydrogenic target atom of charge Z_t, is captured into a given n', l', m' state of a bare projectile ion of charge Z_p. We assume that the time which the projectile spends in the vicinity of the target nucleus is small compared with the transition time of the electron. Let $\vec{r}$, $\vec{r}_t = \vec{r} + \alpha\vec{R}$, and $\vec{r}_p = \vec{r} - (1-\alpha)\vec{R}$ denote the position of the electron with respect to the center of mass, the target nucleus, and the projectile nucleus, respectively, with $\alpha = M_p/(M_p + M_t)$. The projectile is supposed to move rectilinearly and that its trajectory is given by $\vec{R}(t) = \vec{b} + \vec{v}t$ ($\vec{b}\cdot\vec{v} = 0$, $|\vec{b}|$ being the classical impact parameter) with respect to the target nucleus. The cross section can then be written as[7]

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

where the exact eikonal transition amplitude is, in its "prior" form, given by

$$A_{nlm\text{-}n'l'm'}(\vec{b}, v) = -i\int_{-\infty}^{\infty}\left\langle \Psi^{(-)}_{n'l'm'}\left| -\frac{Z_p}{r_p}\right|\psi_{nlm}\right\rangle dt\,, \quad (2)$$

with the time-dependent wave functions

$$\psi_{nlm} = \varphi_{nlm}(\vec{r}_t)\exp(-i\epsilon_p t)\exp(-i\alpha\vec{v}\cdot\vec{r} - \tfrac{1}{2}i\alpha^2v^2t) \quad (3)$$

and

$$\Psi^{(-)}_{n'l'm'} \cong \varphi_{n'l'm'}(\vec{r}_p)\exp(-i\epsilon_p t) \times \exp[i(1-\alpha)\vec{v}\cdot\vec{r} - \tfrac{1}{2}i(1-\alpha)^2 v^2 t] \times \exp\left(-i\int_t^\infty \frac{Z'_t}{r_t}\,dt'\right). \quad (4)$$

Here, we have introduced the hydrogenic wave functions $\varphi_{nlm}(\vec{r}_t)$ and $\varphi_{n'l'm'}(\vec{r}_p)$, and their eigenenergies $\epsilon_t = -\frac{1}{2}Z_t^2/n^2$ and $\epsilon_p = -\frac{1}{2}Z_p^2/n'^2$ (atomic units are used throughout). Furthermore, the translation factors and the eikonal phase factor are included in the wave functions. The effective target charge Z'_t has been introduced in the final state allowing $Z_t \neq Z'_t$ for multielectron effects. It is associated with the interaction between the target nucleus and the captured electron. We could also obtain the OBK results by setting $Z'_t = 0$ (see the Appendix). The approach being used here to obtain the cross section in a closed form is very much the same as that developed in Ref. 3. First, we employ the integral representation of Gau and Macek for the eikonal phase factor,[8] namely,

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

with $\eta = 1/v$ and introduce two Fourier transforms $G_{nlm}(\vec{p})$ and $g_{n'l'm'}(\vec{q})$ by the relations

$$G_{nlm}(\vec{p}) = (2\pi)^{-3/2}\int \varphi_{nlm}(\vec{r}_t)\left(\frac{1}{\Gamma(-i\eta Z'_t)}\int_0^\infty \lambda^{-i\eta Z'_t-1}\exp[-\lambda(r_t - z_t)]d\lambda\right)\exp(i\vec{p}\cdot\vec{r}_t)d^3r_t \quad (6)$$

and

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

We can, after introducing G_{nlm} and $g_{n'l'm'}$ into the momentum version of the integral (2) and some manipulations involving the Dirac delta function, then reduce a six-dimensional integral (1) to a two-dimensional integral, over a two-dimensional momentum space which is normal to the incident velocity $\vec{v}$

$$\sigma_{nlm \to n'l'm'}(v) = \frac{2^4\pi^4 Z_p^2}{v^2}\int [\,|g_{n'l'm'}(\vec{p}+\vec{v})|^2 |G_{nlm}(\vec{p})|^2]_{p_z = p_{0z}}\, d^2p_b\,, \quad (8)$$

where $p_{0z} = -\frac{1}{2}v + \eta\epsilon$ with $\epsilon = \epsilon_p - \epsilon_t$. We shall proceed to evaluate the integrals $g_{n'l'm'}(\vec{q})$, $G_{nlm}(\vec{p})$, and, finally, $\sigma_{nlm\to n'l'm'}$ in the remainder of this section. With the help of the Schrödinger equation for a hydrogenic system, the quantity $g_{n'l'm'}(\vec{q})$ becomes[7]

$$g_{n'l'm'}(\vec{q}) = \frac{q^2 + q_{n'}^2}{2Z_p}\tilde{\varphi}_{n'l'm'}(\vec{q})\,, \quad (9)$$

where $q_{n'} = Z_p/n'$ and the Fourier transform of the hydrogenic wave function $\tilde{\varphi}_{n'l'm'}(\vec{q})$ is given in closed form,[9] namely,

$$\tilde{\varphi}_{n'l'm'}(\vec{q}) = \frac{4q_{n'}^{5/2}}{(q^2+q_{n'}^2)^2}N_{n'l'}\sin^{l'}\alpha\, C^{l'+1}_{n'-l'-1}(\cos\alpha)\,Y_{l'm'}(\hat{q})\,, \quad (10)$$

with $\hat{q}$ denoting the polar angle $\theta_{\vec{q}}$ and azimuthal angle $\phi_{\vec{q}}$ of the vector $\vec{q}$,

$$N_{n'l'}^2 = \frac{n'(n'-l'-1)(l'!)^2 2^{2l'+1}}{(n'+l')!\,\pi}\,,$$

$$\sin\alpha = \frac{2qq_{n'}}{q^2+q_{n'}^2}\,,$$

and

$$\cos\alpha = \frac{q_{n'}^2 - q^2}{q_{n'}^2 + q^2}\,.$$

Here $C^{\nu}_{\mu}(x)$ is the Gegenbauer polynomial[10] and $Y_{l'm'}(\hat{q})$ the spherical harmonic function.[11] For later use, we further express $C^{l'+1}_{n'-l'-1}(\cos\alpha)$ and $Y_{l'm'}(\hat{q})$ as finite polynomials, i.e.,[12]

$$C_{n'-l'-1}^{l'+1}(\cos\alpha)=\frac{(n'+l')!}{(n'-l'-1)!\,(2l'+1)!}\,{}_2F_1\left(n'+l'+1,\ -n'+l'+1;l'+\tfrac{3}{2};\ \frac{q^2}{q^2+q_{n'}^2}\right)$$

$$=\frac{(n'+l')!}{(n'-l'-1)!\,(2l'+1)!}\sum_{k}^{n'-l'-1}\frac{(n'+l'+1)_k(-n'+l'+1)_k}{(l'+\frac{3}{2})_k k!}\frac{q^{2k}}{(q^2+q_{n'}^2)^k} \tag{11}$$

and[11]

$$Y_{l'm'}(\hat{q})=\left(\frac{(2l+1)(l'-|m'|)!}{4\pi(l'+|m'|)!}\right)^{1/2}P_{l'}^{|m'|}(\cos\theta_{\vec{q}})\exp(im'\phi_{\vec{q}})\times\begin{cases}1 & \text{for } m'\geq 0\\ (-1)^{|m'|} & \text{for } m<0\end{cases} \tag{12}$$

with the associated Legendre function $P_{l'}^{|m'|}(x)$ in the form

$$\frac{(-1)^{|m'|}}{2^{l'}l'!}(1-x^2)^{|m'|/2}\sum_{\substack{\mu=0\\ l'-|m'|\geq 2\mu}}^{l'}(-1)^{\mu}\binom{l'}{\mu}\frac{(2l'-2\mu)!}{(l'-|m'|-2\mu)!}\,x^{l'-|m'|-2\mu}, \tag{13}$$

and $(a)_k=\Gamma(a+k)/\Gamma(a)$ the Pochhammer symbol defined for nonintegers via the gamma function $\Gamma(x)$. The quantity $g_{n'l'm'}(\vec{p}+\vec{v})$ therefore can be written as a finite polynomial

$$g_{n'l'm'}(\vec{p}+\vec{v})=\frac{2^{l'+1/2}q_{n'}^{l'+3/2}}{\pi}\left(\frac{(n'+l')!\,(2l'+1)(l'-|m'|)!}{n'(n'-l'-1)!\,(l'+|m'|)!}\right)^{1/2}\frac{1}{(2l'+1)!}$$

$$\times\sum_{k=0}^{n'-l'-1}\sum_{\mu=0}^{(l'-|m'|)/2}K_k(n',l')H_\mu(l',m')(p_{0z}+v)^{l'-|m'|-2\mu}p_b^{|m'|}[p_b^2+(p_{0z}+v)^2+q_{n'}^2]^{-l'-k-1}$$

$$\times[p_b^2+(p_{0z}+v)^2]^{k+\mu}\times\begin{cases}(-1)^{|m'|} & \text{for } m'\geq 0\\ 1 & \text{for } m'<0\end{cases} \tag{14}$$

where $[a]$ denotes the integral part of the real number a,

$$K_k(n',l')=\frac{(n'+l'+1)_k(-n'+l'+1)_k}{(l'+\frac{3}{2})_k k!},$$

and

$$H_\mu(l',m')=(-1)^\mu\binom{l'}{\mu}\frac{(2l'-2\mu)!}{(l'-|m'|-2\mu)!}.$$

Next, we compute the integral $G_{n'l'm'}(\vec{p})$, i.e., Eq. (6). Inverting the order of integration results in

$$G_{nlm}(\vec{p})=\frac{1}{\Gamma(-i\eta Z_t')}\int_0^\infty \lambda^{-i\eta Z_t'-1}h_{nlm}(\vec{p},\lambda)d\lambda, \tag{15}$$

where

$$h_{nlm}(\vec{p},\lambda)=(2\pi)^{-3/2}\int\varphi_{nlm}(\vec{r}_t)\exp[-\lambda(r_t-z_t)]\times\exp(i\vec{p}\cdot\vec{r}_t)d^3r_t. \tag{16}$$

Furthermore, we define a complex vector

$$\vec{K}\equiv\vec{p}-i\lambda\hat{z}$$

and use the relation

$$\varphi_{nlm}(\vec{r}_t)=R_{nl}(r_t)\,Y_{lm}(\hat{r}_t), \tag{17a}$$

where the radial part is given explicitly by[13]

$$R_{nl}(r_t)=\left(2\frac{Z_t}{n}\right)^{l+3/2}\left(\frac{(n-l-1)!}{2n(n+l)!}\right)^{1/2}\times\sum^{n-l-1}S_\sigma(n,l)\left(2\frac{Z_t}{n}\right)^\sigma\exp\left(-\frac{Z_t}{n}r_t\right)r_t^{l+\sigma}, \tag{17b}$$

with

$$S_\sigma(n,l)=(-1)^\sigma\frac{(n+l)!}{(n-l-1-\sigma)!\,(2l+1+\sigma)!\,\sigma!}.$$

We also have

$$\exp(i\vec{K}\cdot\vec{r}_t)=4\pi\sum_{L=0}^{\infty}\sum_{M=-L}^{L}i^Lj_L(Kr_t)Y_{LM}(\hat{K})\,Y_{LM}^*(\hat{r}_t), \tag{18}$$

where $j_L(Kr_t)$ is the spherical Bessel function but with complex argument, since

$$K=(p^2-2i\lambda p_z-\lambda^2)^{1/2}. \tag{19}$$

Inserting Eqs. (17a) and (18) in Eq. (16), the orthonormality of spherical harmonic functions gives

$$h_{nlm}(\vec{p},\lambda)=i\left(\frac{2}{\pi}\right)^{1/2}Y_{lm}(\hat{K})\times\int_0^\infty R_{nl}(r_t)\exp(-\lambda r_t)j_l(Kr_t)r_t^2dr_t. \tag{20}$$

The use of the explicit form for $R_{nl}(r_t)$ enables one to carry out the r_t integral (20) easily. Furthermore, expressing $Y_{lm}(\hat{K})$ in the same way as when evaluating $g_{n'l'm'}$ in a finite polynomial, permits us to perform the λ integration for the integral $G_{nlm}(\vec{p})$. Notice that because the vector $\vec{K}$ is complex we have $\cos\theta_{\vec{K}} = p_z - i\lambda/(p^2 - 2i\lambda p_z - \lambda^2)^{1/2}$ and $\tan\Phi_{\vec{K}} = p_y/p_x$, where $\Phi_{\vec{K}}$ is independent of λ. We find then that

$$G_{nlm}(\vec{p}) = \frac{2i^l}{\Gamma(-i\eta Z_t')} \left(\frac{Z_t}{n}\right)^{l+3/2} \left(\frac{(n-l-1)!\,(2l+1)!\,(l-|m|)!}{2n(n+l)!\,4\pi(l+|m|)!}\right)^{1/2} \frac{(-1)^{|m|}}{2^l l!} \left(2\frac{Z_t}{n} - 2ip_{0z}\right)^{i\eta Z_t'} \left(p^2 + \frac{Z_t^2}{n^2}\right)^{-i\eta Z_t'}$$

$$\times \Bigg[\sum_{\sigma=0}^{n-l-1} \sum_{\nu=0}^{(\sigma+1)/2} \sum_{\tau=0}^{(l-|m|)/2} \sum_{\gamma=0}^{\tau+\nu} \sum_{\delta=0}^{l-|m|-2\tau+2\gamma} \sum_{\alpha=0}^{\sigma+1-2\nu} S_\sigma(n,l) N_\nu(l,\sigma)\, T_\tau(l,m)\, M_\gamma(\nu,\tau)\, D_\delta(\tau,\gamma) A_\alpha(\sigma,\nu)$$

$$\times (-i)^\delta 2^\sigma \frac{\Gamma(2l+\sigma+3)}{\Gamma(l+3/2)} \left(\frac{Z_t}{n}\right)^{2\sigma+1-2\nu-\alpha} p_{0z}^{\,l-|m|-2\tau+2\gamma-\delta} \left(2\frac{Z_t}{n} - 2ip_{0z}\right)^{-\delta-\alpha} B(\delta+\alpha-i\eta Z_t',\, l+\sigma+2-\delta-\alpha+i\eta Z_t')$$

$$\times p_b^{|m|+2(\tau+\nu-\gamma)} \left(p^2 + \frac{Z_t^2}{n^2}\right)^{-(l+\sigma+2)+\delta+\alpha} \Bigg] \exp(im\phi_{\vec{p}}) \times \begin{cases} 1 & \text{for } m \geq 0 \\ (-1)^{|m|} & \text{for } m < 0 \end{cases} \tag{21}$$

where

$$S_\sigma(n,l) = (-1)^\sigma \frac{(n+l)!}{(n-l-1-\sigma)!\,(2l+1+\sigma)!\,\sigma!},$$

$$N_\nu(l,\sigma) = (-1)^\nu \frac{[(-\sigma-1)/2]_\nu(-\sigma/2)_\nu}{(l+\frac{3}{2})_\nu\,\nu!},$$

$$T_\tau(l,m) = (-1)^\tau \frac{l!\,(2l-2\tau)!}{\tau!\,(l-\tau)!\,(l-|m|-2\tau)!},$$

$$M_\gamma(\nu,\tau) = \frac{(\tau+\nu)!}{\gamma!\,(\tau+\nu+\gamma)!},$$

$$D_\delta(\tau,\gamma) = \frac{(l-|m|-2\tau+2\gamma)!}{\delta!\,(l-|m|-2\tau+2\gamma-\delta)!},$$

$$A_\alpha(\sigma,\nu) = \frac{(\sigma+1-2\nu)!}{\alpha!\,(\sigma+1-2\nu-\alpha)!},$$

$$\tan\phi_{\vec{p}} = \frac{p_y}{p_x},$$

and $B(x,y)$ is the usual beta function,[14] defined by

$$B(x,y) \equiv \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)},$$

with x and y complex in the present case. We remark, for the case of the hydrogenic target, that the following equality holds, namely,

$$(p_{0z}+v)^2 + \frac{Z_p^2}{n'^2} = p_{0z}^2 + \frac{Z_t^2}{n^2} \tag{22}$$

because $\epsilon = -\frac{1}{2}Z_p^2/n'^2 - (-\frac{1}{2}Z_t^2/n^2)$. Combining Eqs. (14) and (21), and inserting in Eq. (8), the integral over $\vec{p}_b$ may be done immediately via[15]

$$\int_0^\infty x^{\lambda-1}(1+x)^{-\mu+\nu}(x+\beta)^{-\nu}dx = B(\mu-\lambda,\lambda)\,{}_2F_1(\nu,\mu-\lambda;\mu;1-\beta).$$

The resulting expression for the cross section is

$$
\begin{aligned}
\sigma_{nlm-n'l'm'}(v) = {} & \sigma^{\mathrm{OBK}}_{n-n'} 2^{-4}(5)\pi \frac{1}{|\Gamma(-i\eta Z_t')|^2} \exp\left[-2\eta Z_t' \tan^{-1}\left(-\frac{np_{0z}}{Z_t}\right)\right]\left(\frac{Z_p}{n'}\right)^{2l'} \frac{2^{2l'}(n'+l')!(2l'+1)(l'-|m'|)!}{n'(n'-l'-1)![(2l'+1)!]^2(l'+|m'|)!}\left(\frac{Z_t}{n}\right)^{2l} \\
& \times \frac{(n-l-1)!(2l+1)(l-|m|)!}{n(n+l)!2^{2l}(l!)^2(l+|m|)!}(p_{0z}+v)^{2(l'-|m'|)} p_{0z}^{2(l-|m|)} \\
& \times \sum_{k,k'=0}^{n'-l'-1} \sum_{\mu,\mu'=0}^{[(l'-|m'|)/2]} \sum_{\sigma,\sigma'=0}^{n-l-1} \sum_{\nu,\nu'=0}^{(\sigma+1)/2,\,(\sigma'+1)/2} \sum_{\tau,\tau'=0}^{(l-|m|)/2} \sum_{\gamma,\gamma'=0}^{\tau+\nu,\,\tau'+\nu'} \sum_{\delta,\delta'=0}^{l-|m|-2\tau+2\gamma,\, l-|m|-2\tau'+2\gamma'} \sum_{\alpha,\alpha'=0}^{\sigma+1-2\nu,\,\sigma'+1-2\nu'} \\
& \qquad \times K_k(n',l')K_{k'}(n',l')H_\mu(l',m')H_{\mu'}(l',m')\, S_\sigma(n,l)S_{\sigma'}(n,l)N_\nu(l,\sigma)N_{\nu'}(l,\sigma')T_\tau(l,m) \\
& \qquad \times T_{\tau'}(l,m)M_\gamma(\nu,\tau)M_{\gamma'}(\nu',\tau')D_\delta(\tau,\gamma)D_{\delta'}(\tau',\gamma')A_\alpha(\sigma,\nu)A_{\alpha'}(\sigma',\nu')(-i)^\delta i^\delta 2^{\sigma+\sigma'} \\
& \qquad \times \frac{\Gamma(2l+\sigma+3)\Gamma(2l+\sigma'+3)}{[\Gamma(l+\frac{3}{2})]^2}\left(\frac{Z_t}{n}\right)^{2\sigma+2\sigma'-2\nu-2\nu'-\alpha-\alpha'}(p_{0z}+v)^{2k+2k'} p_{0z}^{-2\tau-2\tau'+2\gamma+2\gamma'-\delta-\delta'} \\
& \qquad \times \left(2\frac{Z_t}{n}-2ip_{0z}\right)^{-\delta-\alpha}\left(2\frac{Z_t}{n}+2ip_{0z}\right)^{-\delta'-\alpha'} B(\delta+\alpha-i\eta Z_t',\, l+\sigma+2-\delta-\alpha+i\eta Z_t') \\
& \times B(\delta'+\alpha'+i\eta Z_t',\, l+\sigma'+2-\delta'-\alpha'-i\eta Z_t')\left(p_{0z}^2+\frac{Z_t^2}{n^2}\right)^{a+b-c+5} B(c-b,b)\,{}_2F_1\left(a,b;c;1-\frac{p_{0z}^2+Z_t^2/n^2}{(p_{0z}+v)^2}\right),
\end{aligned}
\tag{23}
$$

with

$$a = -(k+k'+\mu+\mu'),$$

$$b = |m| + |m'| + \nu + \nu' + \tau + \tau' - \gamma - \gamma' + 1,$$

and

$$c = 2l + 2l' + \sigma + \sigma' - \alpha - \alpha' - \delta - \delta' - \mu - \mu' + 6,$$

where

$$\sigma^{\mathrm{OBK}}_{n-n'}(v) = \frac{2^8 \pi Z_t^5 Z_p^5}{5v^2 n^5 n'^3}\left(p_{0z}^2 + \frac{Z_t^2}{n^2}\right)^{-5}$$

is the OBK result for capture from the nth shell of the target to the n'th shell of the projectile. In particular, the capture cross section for the $1s-(n',l',m')$ is of current interest and is rather simple, namely,

$$
\begin{aligned}
\sigma_{1s-n'l'm'}(v) = {} & \sigma^{\mathrm{OBK}}_{1s-n'}(v)(5)\frac{\pi\eta Z_t'}{\sinh(\pi\eta Z_t')}\exp\left[-2\eta Z_t'\tan^{-1}\left(\frac{-p_{0z}}{Z_t}\right)\right]\frac{(n'+l')!(2l'+1)2^{2l'}}{n'(n'-l'-1)![(2l'+1)!]^2}\frac{(l'-|m'|)!}{(l'+|m'|)!}\left(\frac{Z_p}{n'}\right)^{2l'} \\
& \times (p_{0z}+v)^{2l-2|m'|}\sum_{j=1}^{3}\sum_{k,k'=0}^{n'-l'-1}\sum_{\mu,\mu'=0}^{(l'-|m'|)/2} C_j K_k(n',l')K_{k'}(n',l')H_\mu(l',m')H_{\mu'}(l',m') \\
& \qquad \times (p_{0z}+v)^{2k+2k'}(p_{0z}^2+Z_t^2)^{-2l'-k-k'+|m'|-j+3} \\
& \qquad \times {}_2F_1\left(-k-k'-\mu-\mu',|m'|+1;2l'+j-\mu-\mu'+3;1-\frac{p_{0z}^2+Z_t^2}{(p_{0z}+v)^2}\right),
\end{aligned}
\tag{24}
$$

where

$$C_1 = \frac{\eta^2 Z_t'^2}{4Z_t^2(p_{0z}^2+Z_t^2)},$$

$$C_2 = \frac{\eta Z_t'(p_{0z}-\eta Z_t' Z_t)}{Z_t(p_{0z}^2+Z_t^2)},$$

and

$$C_3 = 1 + \eta^2 Z_t'^2.$$

III. RESULTS AND DISCUSSION

In Sec. II we managed to obtain a closed form for the most general capture process, i.e., $(n,l,m)-(n', l', m')$ transition for the bare projectile-hydrogenic target system. Because of the complexity of the results, we have checked several special cases. For example, we summed over the final m' level for a specific n' and l' and compared the resulting expressions with that obtained previously[1,2] for the transitions $1s$-$2s$, $1s$-$2s$, $1s$-$2p$, and $1s$-$3d$; moreover, we compared our calculations with those done independently for the separate transitions, i.e., $2s-(n',l',m')$ and $2p\pm 1, 0-(n',l',m')$. For all of these comparisons, complete agreement has been obtained. As mentioned in Sec. I, we are particularly interested in the case where the distinct final sublevels m' could possibly be experimentally distinguished in the near future,[4,5] i.e., specifically, the transitions $Z_p + \mathrm{H}(1s) \rightarrow (Z_p+e^-)_{n'l'm'} + \mathrm{H}^+$ for all $n'=2,3$ states. The cross sections of these specific processes are as follows:

$$\sigma_{1s-2p0}(v)=\sigma^{\mathrm{OBK}}_{1-2}(v)\mathfrak{F}(\eta Z_t',Z_t,p_{0z})(5)Z_p^2(p_{0z}+v)^2\sum_{j=1}^{3}C_j\frac{A^{1-j}}{(4+j)}, \tag{25a}$$

$$\sigma_{1s-2p\pm1}(v)=\sigma^{\mathrm{OBK}}_{1-2}(v)\mathfrak{F}(\eta Z_t',Z_t,p_{0z})\tfrac{5}{2}Z_p^2\sum_{j=1}^{3}C_j\frac{A^{2-j}}{(4+j)(3+j)}, \tag{25b}$$

$$\sigma_{1s-3s}(v)=\sigma^{\mathrm{OBK}}_{1-3}(v)\mathfrak{F}(nZ',Z_t,p_{0z})(5)\sum_{j=1}^{3}C_jA^{-j}\left[\frac{A^3}{(2+j)}-\frac{2^5}{3}\left(\frac{Z_p}{3}\right)^2\frac{A^2}{(3+j)}+\frac{(11)2^5}{9}\left(\frac{Z_p}{3}\right)^4\frac{A}{(4+j)}\right.$$
$$\left.-\frac{2^9}{9}\left(\frac{Z_p}{3}\right)^6\frac{1}{(5+j)}+\frac{2^8}{9}\left(\frac{Z_p}{3}\right)^8\frac{A^{-1}}{(6+j)}\right], \tag{25c}$$

$$\sigma_{1s-3p0}(v)=\sigma^{\mathrm{OBK}}_{1-3}(v)\mathfrak{F}(\eta Z_t',Z_t,p_{0z})\frac{(5)2^5}{3}\left(\frac{Z_p}{3}\right)^2\sum_{j=1}^{3}C_jA^{-j}\left[\frac{A^2}{(3+j)}-5\left(\frac{Z_p}{3}\right)^2\frac{A}{(4+j)}+8\left(\frac{Z_p}{3}\right)^4\frac{1}{(5+j)}\right.$$
$$\left.-4\left(\frac{Z_p}{3}\right)^6\frac{A^{-1}}{(6+j)}\right], \tag{25d}$$

$$\sigma_{1s-3p\pm1}(v)=\sigma^{\mathrm{OBK}}_{1-3}(v)\mathfrak{F}(\eta Z_t',Z_t,p_{0z})\frac{(5)2^4}{3}\left(\frac{Z_p}{3}\right)^2\sum_{j=1}^{3}C_jA^{-j}\left[\frac{A^2}{(4+j)(3+j)}-4\left(\frac{Z_p}{3}\right)^2\frac{A}{(5+j)(4+j)}\right.$$
$$\left.+4\left(\frac{Z_p}{3}\right)^4\frac{1}{(6+j)(5+j)}\right], \tag{25e}$$

$$\sigma_{1s-3d0}(v)=\sigma^{\mathrm{OBK}}_{1-3}(v)\mathfrak{F}(\eta Z_t',Z_t,p_{0z})\frac{(5)2^7}{9}\left(\frac{Z_p}{3}\right)^4\sum_{j=1}^{3}C_jA^{-j}\left(\frac{1}{2}\frac{A}{(6+j)(5+j)(4+j)}-\frac{p_{0z}+v}{(6+j)(5+j)}+\frac{(p_{0z}+v)^2A^{-1}}{(6+j)}\right), \tag{25f}$$

$$\sigma_{1s-3d\pm1}(v)=\sigma^{\mathrm{OBK}}_{1-3}(v)\mathfrak{F}(\eta Z_t',Z_t,p_{0z})\frac{(5)2^6}{3}\left(\frac{Z_p}{3}\right)^4(p_{0z}+v)\sum_{j=1}^{3}C_j\frac{A^{-j}}{(6+j)(5+j)}, \tag{25g}$$

and

$$\sigma_{1s-3d\pm2}(v)=\sigma^{\mathrm{OBK}}_{1-3}(v)\mathfrak{F}(\eta Z_t',Z_t,p_{0z})\frac{(5)2^5}{3}\left(\frac{Z_p}{3}\right)^4\sum_{j=1}^{3}C_j\frac{A^{1-j}}{(6+j)(5+j)(4+j)}, \tag{25h}$$

where

$$\mathfrak{F}(\eta Z_t',Z_t,p_{0z})=\frac{\pi\eta Z_t'}{\sinh(\pi\eta z_t')}\exp\left[-2\eta Z_t'\tan^{-1}\left(\frac{-p_{0z}}{Z_t}\right)\right],$$

and

$$A=p_{0z}^2+Z_t^2.$$

In Table I, we have listed numerically the capture cross sections of the collision processes $\mathrm{H}^+ + \mathrm{H}(1s) \rightarrow \mathrm{H}(n',l',m') + \mathrm{H}^+$ with $n'=2$ and 3 for the proton energy ranging from 25 to 200 keV in both the eikonal and OBK calculations. Furthermore, to see the relative roles played by distinct final n', l', m' sublevels, we have also plotted these cross sections, as a function of the proton energy, in Figs. 1 and 2. We notice that the eikonal result is several times smaller than its OBK counterpart for all these transitions. The curvatures of both eikonal and OBK curves (the cross section versus the collision energy) for a specific transition are very much alike except the two curves come a little bit closer as the energy

TABLE I. Calculated charge capture cross sections $\sigma_{1s \to n'l'm'}$ (in 10^{-16} cm^2) for the reactions $H^+ + H(1s) \to H(n'l'm') + H^+$, with $n' = 2$ and 3, as a function of energy. The results for both eikonal (denoted by a) and OBK (denoted by b) are tabulated.

E_i (keV/amu)	25	50	75	100	150	200
$n'l'm'$						
2 0 0	[a]3.88(−1)	9.55(−2)	3.20(−2)	1.28(−2)	2.90(−3)	8.92(−4)
	[b]1.84	4.93(−1)	1.62(−1)	6.27(−2)	1.33(−2)	3.87(−3)
2 1 0	6.10(−1)	1.12(−1)	2.80(−2)	8.83(−3)	1.39(−3)	3.25(−4)
	2.76	5.44(−1)	1.33(−1)	4.07(−2)	6.00(−3)	1.33(−3)
2 1 1	6.20(−2)	1.05(−2)	2.49(−3)	7.56(−4)	1.14(−4)	2.59(−5)
	3.05(−1)	5.73(−2)	1.35(−2)	3.99(−3)	5.66(−4)	1.23(−4)
3 0 0	1.35(−1)	3.26(−2)	1.07(−2)	4.23(−3)	9.40(−4)	2.85(−4)
	5.12	1.52(−1)	5.09(−2)	1.98(−2)	4.19(−3)	1.21(−3)
3 1 0	2.17(−1)	4.23(−2)	1.07(−2)	3.35(−3)	5.23(−4)	1.21(−4)
	8.01(−1)	1.86(−1)	4.78(−2)	1.48(−2)	2.20(−3)	4.87(−4)
3 1 1	2.04(−2)	3.70(−3)	8.93(−4)	2.73(−4)	4.11(−5)	9.34(−6)
	8.04(−2)	1.82(−2)	4.54(−3)	1.38(−3)	1.99(−4)	4.34(−5)
3 2 0	3.05(−2)	4.98(−3)	1.01(−3)	2.64(−4)	3.03(−5)	5.54(−6)
	1.10(−1)	2.12(−2)	4.38(−3)	1.12(−3)	1.23(−4)	2.14(−5)
3 2 1	6.92(−3)	1.08(−3)	2.14(−4)	5.46(−5)	6.11(−6)	1.10(−6)
	2.65(−2)	5.04(−3)	1.02(−3)	2.58(−4)	2.77(−5)	4.77(−6)
3 2 2	5.28(−4)	7.77(−5)	1.49(−5)	3.71(−6)	4.05(−7)	7.19(−8)
	2.13(−3)	3.98(−4)	7.94(−5)	1.98(−5)	2.09(−6)	3.56(−7)

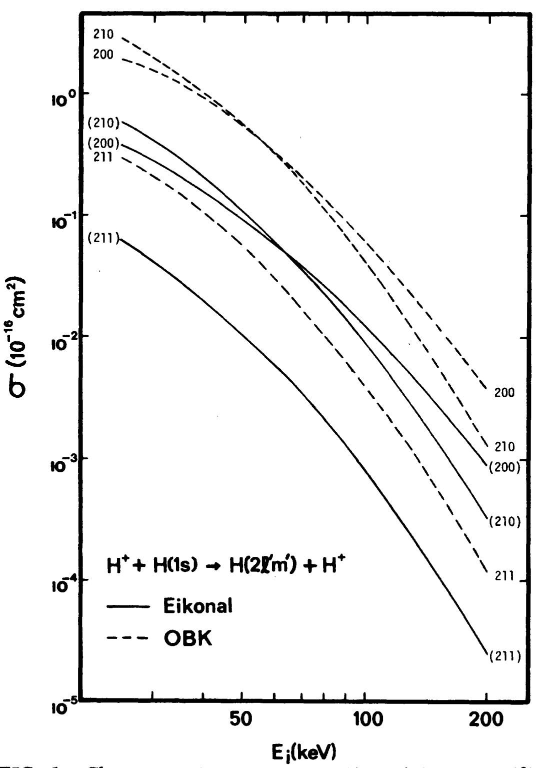

FIG. 1. Charge capture cross sections into a specified $n' = 2, l', m'$ shell of the impact proton from the K shell of a hydrogen atom, i.e., $H^+ + H(1s) \to H(n' = 2, l', m') + H^+$, as a function of the impact energy. Solid curves are the eikonal calculations while dashed curves are the OBK calculations. Each curve is indexed at both ends by a set of three digits representing the hydrogenic quantum numbers n', l', and m', respectively.

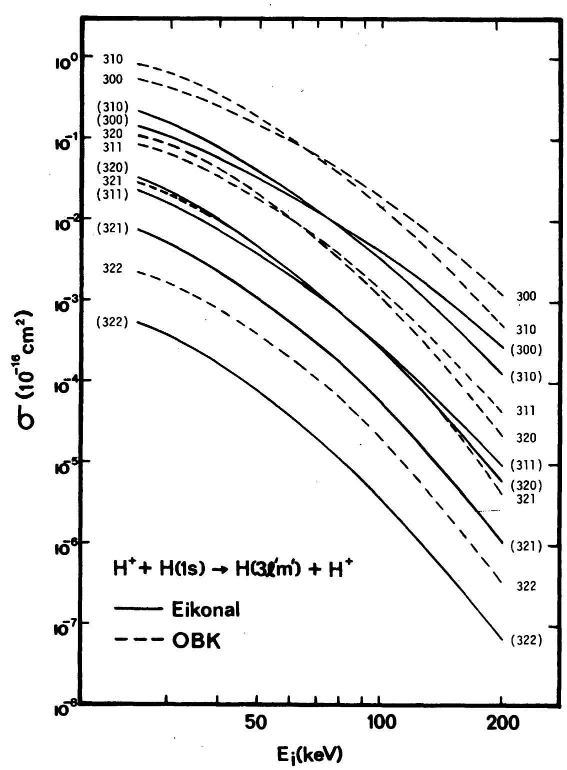

FIG. 2. Charge capture cross sections for the process $H^+ + H(1s) \to H(n' = 3, l', m') + H^+$ as a function of the impact energy. Solid curves are the eikonal calculations while dashed curves are the OBK calculations. Each curve is indexed at both ends by a set of three digits representing the hydrogenic quantum numbers n', l', and m', respectively.

increases.

In conclusion, we would like to point out that although our final expression $\sigma_{nlm\to n'l'm'}(v)$ of Eq. (23) is the most general result and is exact within the eikonal approximation, no direct experimental verification involving the m' (magnetic quantum state) contribution has been reported yet. Since previous eikonal theoretical results[1-3] which are special cases of our present results agree well with existing experimental data, we have confidence in the theory presented in this paper. Detailed experimental measurement is needed to test the limitations of the general eikonal approach and therefore would be of great value.

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APPENDIX: THE OBK FORMULA FOR $\sigma_{nlm-n'l'm'}(v)$

The OBK result which corresponds to our exact eikonal form has been previously obtained by Sil[16] only for the $n=1$ initial target state. By simply setting $Z_t'=0$ in our result, Eq. (23), the general OBK result may be obtained. Because of the complexity of that formula, we present here a simple and more transparent derivation of the OBK result. It should be noted that the OBK result has ten finite summations, whereas the eikonal result has 17, counting the hypergeometric function in each case.

We recall Eq. (8), namely,

$$\sigma_{nlm\to n'l'm'}(v)=\frac{2^4\pi^4 Z_p^4}{v^2}\int [\,|g_{n'l'm'}(\vec{p}+\vec{v})|^2 |G_{nlm}(\vec{p})|^2]_{p_z=p_{0z}}\, d^2p_b\,. \tag{A1}$$

Notice that $G_{nlm}(\vec{p})$ in this case is just the Fourier transform of the spatial representation of the hydrogenic wave function $\varphi_{nlm}(\vec{r}_t)$, i.e.,

$$G_{nlm}(\vec{p})=(2\pi)^{-3/2}\int \varphi_{nlm}(\vec{r}_t)e^{i\vec{p}\cdot\vec{r}_t}d^3r_t\ , \tag{A2}$$

which has been expressed in a closed form, Eq. (10), while $g_{n'l'm'}(\vec{p}+\vec{v})$ is the same as before, Eq. (14). Substituting G_{nlm} and $g_{n'l'm'}$ in Eq. (A1) after some manipulations, gives

$$\begin{aligned}\sigma^{\mathrm{OBK}}_{nlm-n'l'm'}(v)=\sigma^{\mathrm{OBK}}_{n-n'}\cdot 5\cdot 2^{2l'}\left(\frac{Z_p}{n'}\right)^{2l'}&\frac{(n'+l')!(2l+1)}{n'(n'-l'-1)![(2l'+1)!]^2}\,\frac{(l'-|m'|)!}{(l'+|m'|)!}\,2^{2l}\left(\frac{Z_t}{n}\right)^{2l}\frac{n(n+l)!(2l+1)}{(n-l-1)![(2l+1)!]^2}\\ &\times\frac{(l-|m|)!}{(l+|m|)!}\sum_{k,k'=0}^{n'-l'-1}\ \sum_{\mu,\mu'=0}^{(l'-|m'|)/2}\ \sum_{\nu,\nu'=0}^{n-l-1}\ \sum_{\tau,\tau'=0}^{(-l-|m|)/2}\ \sum_{\alpha=0}^{\nu+\nu'+\tau+\tau'} K_k(n',l')K_{k'}(n',l')\\ &\times H_\mu(l',m')H_{\mu'}(l',m')D_\nu(n,l)D_{\nu'}(n,l)\,T_\tau(l,m)T_{\tau'}(l,m)A_\alpha(\nu,\nu';\tau,\tau')\\ &\times(p_{0z}+v)^{2(l'-|m'|+k+k')}p_{0z}^{2(l-|m|+\nu+\nu'-\alpha)}\left(p_{0z}^2+\frac{Z_t^2}{n^2}\right)^{-(2l+2l'+k+k'+\nu+\nu'-|m|-|m'|-\alpha)}\\ &\times B(2l+2l'+\nu+\nu'-\mu-\mu'-|m|-|m'|-\alpha+5,\ |m|+|m'|+\alpha+1)\\ &\times{}_2F_1\left(-k-k'-\mu-\mu',\ |m|+|m'|+\alpha+1;\ 2l+2l'+\nu+\nu'-\mu-\mu'+6;\ 1-\frac{p_{0z}^2+Z_t^2/n^2}{(p_{0z}+v)^2}\right),\end{aligned} \tag{A3}$$

where

$$D_\nu(n,l)=\frac{(n+l+1)_\nu(-n+l+1)_\nu}{(l+\frac{3}{2})_\nu\,\nu!}\,,$$

and

$$A_\alpha(\nu,\nu';\tau,\tau')=\binom{\nu+\nu'+\tau+\tau'}{\alpha}.$$

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