Charge transfer in collisions of atomic hydrogen with N^{7+} ions in the high-energy region

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A method to calculate electron-capture cross sections for collisions between an arbitrary $n_i l_i m_i$ shell of a hydrogenic target and an arbitrary $n_f l_f m_f$ shell of a fast bare projectile has been developed in the framework of the continuum distorted-wave approximation. Analytical expressions are derived for the Coulomb integrals in closed form in terms of Gauss hypergeometric functions in a terminating series. As an application, the cross sections in N⁷⁺ + H(1s) collisions are calculated in the energy range between 10 and 40 MeV and compared with existing theoretical calculations. The total charge-transfer cross sections have been evaluated by applying an n^{-3} law for $n \ge 7$ levels.

I. INTRODUCTION

Charge-transfer processes between fully or partially stripped ions and atomic hydrogen have aroused immense interest in recent years with a focus on processes relevant to magnetically confined fusion plasmas and astrophysical plasmas.¹ Current interest in collisions between heavy fully stripped ions and the ground state of atomic hydrogen is accelerated due to the advent of multiply charged ion sources. Experimental investigations^{2–15} to determine the charge-transfer cross sections for collisions between fully or partially stripped ions and hydrogen have been reported by several workers.

Extensive investigations¹⁶⁻³² have also been made theoretically for collisions of multicharged ions with atomic hydrogen. Olson and Salop¹⁶ applied the classical trajectory Monte Carlo method (CTMC) to calculate the charge-transfer cross sections for collisions between fully or partially stripped ions and the ground-state atomic hydrogen in the intermediate-energy range. The unitarized distorted-wave approximation (UDWA) developed by Ryufuku and Watanabe¹⁷ has been applied to study the collisions of multicharged ions with atomic hydrogen in the low-, intermediate-, and high-energy regions. The cross sections for electron capture between arbitrary hydrogenic states of the target and projectile have been cal-culated by Omidvar¹⁸ in the Oppenheimer-Brinkman-Kramers (OBK) approximation. The full "Born" approx-imation has been applied by Toshima¹⁹ to study a few selected transitions between high-lying states of atomic hydrogen. Recently the charge exchange in fast collisions between arbitrary hydrogenic states nl and n'l' of the target and projectile has been reported by Eichler²⁰ in the eikonal approximation. The eikonal calculations have also been extended by Ho *et al.*²¹ to cover *nlm* contributions.

To study the processes involving multicharged ions, it is now well established³³⁻³⁵ that one should take into account the second-order terms to obtain the correct

high-energy behavior of charge-transfer cross sections. The second-order methods such as the impulse approximation (IA) (Refs. 36-39), the continuum intermediatestate⁴⁰ (CIS) method, and the continuum distortedwave⁴¹ (CDW) method have been proposed in connection with the calculations of charge-transfer cross sections in the high-energy region. The CDW approximation takes proper account of the continuum intermediate states and also allows for the distortion of the bound electrons by the incident and scattered ion, and as such, it is expected to give better results of cross sections involving collisions of highly charged ions with atomic targets. Recently Belkić et al.⁴² have developed a method for the calculation of electron-capture cross sections for collisions between an arbitrary $n_i l_i m_i$ shell of a hydrogenic target atom and an arbitrary $n_f l_f m_f$ shell of a fast hydrogenic projectile in the CDW approximation. Their method is based on expanding the angular momentum state of the hydrogenic orbital in terms of the appropriate parabolic orbitals. Using parabolic coordinates they have finally expressed the CDW scattering amplitude as a linear combination of Lauricella polynomials of three variables. However, this method for the evaluation of cross sections is not quite suitable for numerical computation for large values of principal as well as angular momentum quantum numbers. Very recently, Belkić 43 has developed a method for the evaluation of the Coulomb integrals by the use of spherical coordinates, and expressed the results in a compact form by means of Appell hypergeometric polynomials of two variables.

In the present paper we have developed an alternative method for the evaluation of such Coulomb integrals in closed form in terms of terminating Gauss hypergeometric functions by using spherical coordinates in the framework of the CDW approximation. The present approach is, like the previously published methods,^{42,43} suitable for application to any arbitrary excited state and convenient for numerical computation as well. We have applied this method in the calculation of the charge-transfer cross sec-

1657

tions for the $N^{7+} + H(1s)$ collision in the energy range between 10 and 40 MeV. The calculated cross sections are compared with the previously reported theoretical results of $\hat{E}ichler^{20}$ in the eikonal approximation.

In Sec. II we outline the general expression for the CDWA scattering amplitude for the collision between an arbitrary $n_i l_i m_i$ shell of a hydrogenic target and an arbitrary $n_f l_f m_f$ shell of a fast bare projectile, and show the reduction of the scattering amplitude to a closed analytical form. In Sec. III our numerical calculations are discussed and compared with the existing theoretical calculations. Finally, in Sec. IV, a conclusion of the present investigation is drawn. Atomic units are used throughout the paper unless otherwise stated.

II. THEORY

A. General expression of the CDW cross sections

The prior form of the CDW cross sections $Q_{n_l l_l - n_l l_l}$, averaged over initial and summed over final magnetic substates, for electron capture from an arbitrary $n_i l_i m_i$ shell of a hydrogenic target into an arbitrary $n_f l_f m_f$ shell of a fast hydrogenic projectile, can be written as

$$Q_{n_{i}l_{i}\cdot n_{f}l_{f}}(a_{0}^{2}) = \frac{1}{2l_{i}+1} \frac{1}{\pi} (2\pi v)^{-2} \\ \times \sum_{m_{i},m_{f}} \int d\eta | T_{n_{i}l_{i}m_{i}}^{-}(\underline{\eta})_{n_{f}l_{f}m_{f}} |^{2} .$$
(1)

In the prior version of the CDW theory,²⁷ the transition amplitude is given by

$$T_{n_i l_i m_i \cdot n_f l_f m_f}^{-}(\boldsymbol{\eta}) = -N(v) \mathbf{J} \cdot \mathbf{K} , \qquad (2)$$

with

where

$$\mathbf{J} = \int d\mathbf{x} \exp(i\mathbf{p} \cdot \mathbf{x}) \\ \times [\nabla_x \Phi_{n_i l_i m_i}(\mathbf{x})] {}_1F_1(i\nu_t; 1; i\nu x + i\mathbf{v} \cdot \mathbf{x}) , \qquad (3)$$

$$\mathbf{K} = \int d\mathbf{s} \exp(i\mathbf{q} \cdot \mathbf{s}) \Phi_{n_f l_f m_f}^*(\mathbf{s}) \\ \times \nabla_{s} {}_1 F_1(i\nu_p; \mathbf{l}; ivs + i\mathbf{v} \cdot \mathbf{s}) , \qquad (4)$$

$$N(v) = \Gamma(1 - iv_t)\Gamma(1 - iv_p)\exp\left[\frac{1}{2}\pi(v_p + v_t)\right], \qquad (5)$$

$$\mathbf{p} = -\boldsymbol{\eta} - \left[\frac{\varepsilon_i - \varepsilon_f}{v^2} + \frac{1}{2} \right] \mathbf{v} , \qquad (6)$$

$$\mathbf{q} = \boldsymbol{\eta} + \left[\frac{\varepsilon_i - \varepsilon_f}{v^2} - \frac{1}{2} \right] \mathbf{v} , \qquad (7)$$

$$v_p = Z_p / v \quad , \tag{8}$$

$$v_t = Z_t / v \quad . \tag{9}$$

Here we have introduced the hydrogenic wave functions $\Phi_{n_i l_i m_i}(\mathbf{x})$ and $\Phi_{n_f l_f m_f}(\mathbf{s})$, and the corresponding eigenenergies ε_i , ε_f . Z_i and Z_p are, respectively, the charges of the target and the projectile, and η is the transverse momentum transfer perpendicular to the incident velocity. We recast the J integral making use of the Fourier theorem⁴² as

$$\mathbf{J} = \mathbf{J}_1 - \mathbf{J}_2 , \qquad (10)$$

where

$$\mathbf{J}_{1} = i\mathbf{p}' \int d\mathbf{x} \exp(-i\mathbf{p}' \cdot \mathbf{x}) \Phi_{n_{i}l_{i}m_{i}}(\mathbf{x}) \\ \times {}_{1}F_{1}(i\nu_{t}; 1; i\nu x + i\mathbf{v} \cdot \mathbf{x}) , \qquad (11)$$

$$\mathbf{J}_{2} = \int d\mathbf{x} \exp(-i\mathbf{p}' \cdot \mathbf{x}) \Phi_{n_{i}l_{i}m_{i}}(\mathbf{x})$$

$$\times \nabla_{\mathbf{x} \rightarrow 1} F_{1}(i\mathbf{v}_{i}; 1; iv\mathbf{x} + i\mathbf{y} \cdot \mathbf{x}) , \qquad (12)$$

with

$$\mathbf{p}' = -\mathbf{p} \ . \tag{13}$$

B. Evaluation of the integral J_2

The J_2 integral in Eq. (12) may be expressed as

$$\mathbf{J}_{2} = v \nabla_{v} \int d\mathbf{x} \frac{\exp(-i\mathbf{p}' \cdot \mathbf{x})}{x} \\ \times \Phi_{n_{i}l_{i}m_{i}}(\mathbf{x}) {}_{1}F_{1}(i\nu_{t}; 1; ivx + i\mathbf{v} \cdot \mathbf{x}) , \qquad (14)$$

with p' and v_t taken as parameters independent of v. We use the integral representation of the confluent hypergeometric function⁴³ in Eq. (14) and obtain

$$\mathbf{J}_{2} = v \nabla_{v} \frac{1}{2\pi i} \oint dt \ t^{iv_{t}-1} (t-1)^{-iv_{t}} \chi_{n_{i}l_{i}m_{i}}(\Delta, \mathbf{Q}) , \quad (15)$$

where

$$\chi_{n_i l_i m_i}(\Delta, \mathbf{Q}) = \int d\mathbf{x} \frac{\exp(i\mathbf{Q} \cdot \mathbf{x} - \Delta x)}{x} \Phi_{n_i l_i m_i}(\mathbf{x}) , \quad (16)$$

$$\Delta = -ivt , \qquad (17)$$

$$\mathbf{Q} = -\mathbf{p}' + \mathbf{v}t \quad . \tag{18}$$

The evaluation of $\chi_{n_i l_i m_i}(\Delta, \mathbf{Q})$ in Eq. (16) can be performed following a procedure similar to Datta et al.,²⁵ and we obtain

$$\chi_{n_i l_i m_i}(\Delta, \mathbf{Q}) = -N_{n_i l_i m_i}(n_i + l_i)! 4\pi l_i! (2i)^{l_i} \mathcal{Q}^{l_i} Y_{l_i m_i}(\widehat{\mathbf{Q}}) c^{-(l_i+1)} \xi^{n_i - l_i - 1} C_{n_i - l_i - 1}^{l_i + 1}(\lambda) , \qquad (19)$$

$$\gamma_{n_i} = \mathbf{Z}_t / n_i \quad , \tag{21}$$

$$\xi^2 = d \quad , \tag{22}$$

$$b = (\Delta^2 - \gamma_{n_i}^2 + Q^2)/c , \qquad (24)$$

$$c = Q^2 + (\Delta + \gamma_{n_i})^2$$
, (25)

$$d = [Q^{2} + (\Delta - \gamma_{n_{i}})^{2}]/c , \qquad (26)$$

 $Y_{l_im_i}(\hat{\mathbf{Q}})$ and $C_{n_i-l_i-1}^{l_i+1}(\lambda)$ being, respectively, the spherical harmonics and the Gegenbauer polynomial of degree (n_i-l_i-1) and order (l_i+1) . We use the most suitable representation of the Gegenbauer polynomial by its power-series expansion⁴³ as

$$C_{n_i-l_i-1}^{l_i+1}(\lambda) = \sum_{n_{i1}=0}^{[n_i'/2]} \alpha_{n_{i1}}^{n_i l_i} \lambda_{n_i'}^{n_i'} , \qquad (27)$$

where $[n_i'/2]$ is the largest integer contained in the fraction $n_i'/2$, and

$$\alpha_{n_{i1}}^{n_i l_i} = (-1)^{n_{i1}} 2^{n_{i2}'} (n_{i2} - 1)! / (n_{i1}! n_{i2}'! l_i!) , \qquad (28)$$

$$n_i' = n_i - l_i - 1$$
, (29)

$$n_i = n_{i1} + n_{i2} , (30)$$

$$n_i' = n_{i1}' + n_{i2}' , \qquad (31)$$

$$n_{i1}' = 2n_{i1} \ . \tag{32}$$

1

Substituting Eq. (27) into Eq. (19) we arrive at

$$\begin{aligned} \chi_{n_{i}l_{i}m_{i}}(\Delta,\mathbf{Q}) &= -N_{n_{i}l_{i}m_{i}}(n_{i}+l_{i}) \mid 4\pi l_{i} \mid (2i)^{l_{i}} \\ &\times \sum_{n_{i}1=0}^{\left[n_{i}^{\prime}/2\right]} \alpha_{n_{i}1}^{n_{i}l_{i}} \mathcal{Q}^{l_{i}} Y_{l_{i}m_{i}}(\widehat{\mathbf{Q}}) \mathcal{Q}_{+}^{-n_{i2}} \mathcal{Q}_{-}^{n_{i1}} \mathcal{Q}_{0}^{n_{i'}}, \end{aligned}$$

$$(33)$$

where the quantities
$$Q_0$$
 and Q_{\pm} exhibit a simple t dependence as

$$Q_{-} = a_{-}(1 - \rho t)$$
, (34)

$$Q_0 = a_0(1 - \sigma t) , \qquad (35)$$

$$Q_{+} = a_{+}(1 - \tau t) , \qquad (36)$$

where

$$\rho = 2(\mathbf{p}' \cdot \mathbf{v} - ivb_{-}) , \qquad (37)$$

$$b_{-} = \gamma_{n_i} , \qquad (38)$$

$$a_{-} = p'^{2} + b_{-}^{2} , \qquad (39)$$

$$\sigma = -2\mathbf{p}' \cdot \mathbf{v}/a_0 \quad , \tag{40}$$

$$a_0 = p'^2 - b_-^2 , \qquad (41)$$

$$\tau = 2(\mathbf{p}' \cdot \mathbf{v} + ivb_{-})/a_{+} , \qquad (42)$$

$$a_{+} = p'^{2} + b_{-}^{2} \quad . \tag{43}$$

We use⁴⁴ the addition theorem of regular solid harmonics in an arbitrary quantization axis and get

$$Q^{l_i} Y_{l_i m_i}(\widehat{\mathbf{Q}}) = \sum_{l_i'=0}^{l_i} \sum_{m_i = -l_i'}^{l_i'} N_{l_i' l_i''} t^{l_i'}, \qquad (44)$$

with

$$N_{l_{i}^{\prime}l_{i}^{\prime\prime\prime}} = (-1)^{l_{i}^{\prime\prime}} {}^{(l_{i}^{\prime}+m_{i}^{\prime})} v^{l_{i}^{\prime}} p^{\prime} {}^{l_{i}^{\prime\prime}} Y_{l_{i}^{\prime}m_{i}^{\prime\prime}}(\mathbf{\hat{p}}) Y_{l_{i}^{\prime\prime}m_{i}^{\prime\prime}}(\mathbf{\hat{p}}^{\prime}) \left[\frac{4\pi (l_{i}^{\prime}+\mid m_{i}^{\prime}\mid)! (l_{i}^{\prime\prime}+\mid m_{i}^{\prime\prime}\mid)! (2l_{i}+1)(l_{i}-m_{i})!}{(2l_{i}^{\prime}+1)(l_{i}^{\prime\prime}-\mid m_{i}^{\prime\prime}\mid)! (2l_{i}^{\prime\prime}+1)(l_{i}^{\prime\prime}-\mid m_{i}^{\prime\prime}\mid)! (l_{i}+m_{i})!} \right]^{1/2},$$

$$(45)$$

$$l_{i}^{\prime\prime} = l_{i} - l_{i}^{\prime},$$

$$(46)$$

$$m_i'' = m_i - m_i' \ . \tag{47}$$

Substituting Eqs. (33) and (44) into Eq. (15) and taking the binomial expansion of $Q_{0}^{n'_{2}}$, $Q_{+}^{-n_{i_{2}}}$, and $Q_{-}^{n_{i_{1}}}$, the contour integration of the J_{2} integral in Eq. (15) can be performed following a procedure similar to Saha *et al.*,⁴⁵ and finally we arrive at

$$\mathbf{J}_{2} = -vN_{n_{i}l_{i}m_{i}}(n_{i}+l_{i})!4\pi l_{i}!(2i)'^{i}\mathbf{V}_{v}$$

$$\times \sum_{n_{i}1=0}^{[n_{i}'/2]} \sum_{l_{i}'=0}^{l_{i}} \sum_{m_{i}=-l_{i}'}^{n_{i}} \sum_{\omega_{i}=0}^{n_{i}1} \sum_{\delta_{i}=0}^{n_{i}'} \alpha_{n_{i}1}^{n_{i}l_{i}} N_{l_{i}'l_{i}''}a_{+}^{-n_{i}2}(\frac{n_{i}}{\omega_{i}})\rho'^{\omega_{i}}a_{-}^{n_{i}1-\omega_{i}}(\frac{n_{i}'}{\delta_{i}})\sigma'^{\delta_{i}}a_{0}^{n_{i}'_{2}-\delta_{i}}(i\nu_{i})_{l_{i}'+\omega_{i}+\delta_{i}}$$

 $\times {}_{2}F_{1}(n_{i2}, i\nu_{t} + l_{i}' + \omega_{i} + \delta_{i}, l_{i}' + \omega_{i} + \delta_{i} + 1, \tau'/a_{+})/(l_{i}' + \omega_{i} + \delta_{i})! , \qquad (48)$

where

$$\rho' = -a_{-}\rho , \qquad (49)$$

$$\sigma' = -a_0 \sigma \quad , \tag{50}$$

$$\tau' = a_+ \tau \ . \tag{51}$$

We now apply the ∇_v operator in Eq. (48) and then choose our axis of quantization along the direction of v and arrive at the J_2 integral in a terminating hypergeometric series as

(40)

$$\mathbf{J}_{2} = \sum_{n_{i1}=0}^{[n_{i}'/2]} \sum_{l_{i}'=0}^{l_{i}} \sum_{\omega_{i}=0}^{n_{i1}} \sum_{\delta_{i}=0}^{n_{i2}'} N_{1}(m_{i}'=0)N_{2}(m_{i}'=0)M_{1}(p_{x}'+ip_{y}')^{m_{i}}\mathbf{p}' + N_{i}(m_{i}'=0)N_{2}(m_{i}'=0)M_{2}(p_{x}'+ip_{y}')^{m_{i}}(-\mathbf{p}'+i\gamma_{n_{i}}\mathbf{\hat{v}}) + N_{1}(m_{i}'=0)N_{2}(m_{i}'=0)M_{3}(p_{x}'+ip_{y}')^{m_{i}}(\mathbf{p}'+i\gamma_{n_{i}}\mathbf{\hat{v}}) + N_{1}(m_{i}'=1)N_{2}(m_{i}'=1)M_{4}(p_{x}'+ip_{y}')^{m_{i}-1}(\mathbf{\hat{i}}+i\mathbf{\hat{j}}) + N_{1}(m_{i}'=0)N_{2}(m_{i}'=0)M_{5}(p_{x}'+ip_{y}')^{m_{i}}\mathbf{\hat{k}} + N_{1}(m_{i}'=0)N_{2}(m_{i}'=0)M_{6}(p_{x}'+ip_{y}')^{m_{i}}\mathbf{v},$$
(52)

where

$$N_{1}(m_{i}') = -v N_{n_{i}l_{i}m_{i}}(n_{i}+l_{i})! 4\pi l_{i}!(2i)^{l_{i}} \alpha_{n_{i1}}^{n_{i}l_{i}} N_{l_{i}'l_{i}''} a_{+}^{-n_{i2}} \binom{n_{i1}}{\omega_{i}} a_{-}^{n_{i1}-\omega_{i}} \binom{n_{i2}'}{\delta_{i}} a_{0}^{n_{i2}'-\delta_{i}} (i\nu_{i})_{l_{1}'+\omega_{i}+\delta_{i}} / (l_{i}'+\omega_{i}+\delta_{i})! ,$$

$$(53)$$

$$N_{2}(m_{i}') = N_{yl_{i}''m_{i}''} \sum_{\mathbf{K}=0}^{[(l_{i}''-m_{i}'')/2]} (-1)^{\mathbf{K}} \frac{(2l_{i}''-2\mathbf{K})!}{2^{l_{i}'}(l_{i}''-\mathbf{K})!(l_{i}''-m_{i}''-2\mathbf{K})!\mathbf{K}!} p_{z}'^{l_{i}''-m_{i}''-2\mathbf{K}} p'^{2\mathbf{K}},$$
(54)

$$N_{yl_i''m_i''} = \epsilon \left[\frac{(2l_i''+1)(l_i''-|m_i''|)!}{4\pi(l_i''+|m_i''|)!} \right]^{1/2},$$
(55)

with $\epsilon = (-1)^{m''_i}$ for $m''_i > 0$ and $\epsilon = 1$ for $m''_i \le 0$.

$$M_{1} = -2\delta_{1}(a_{0}\sigma)^{\delta_{i}-1}(-2\rho)^{\omega_{i}}v^{l_{i}'}Y_{l_{i}'0}(\hat{\mathbf{v}})_{2}F_{1}(n_{i2},i\nu_{t}+l_{i}'+\omega_{i}+\delta_{i},l_{i}'+\omega_{i}+\delta_{i}+1,\tau'/a_{+}), \qquad (56)$$

$$M_{2} = 2(a_{0}\sigma)^{\delta_{i}}\omega_{i}(-2\rho)^{\omega_{i}-1}v^{l_{i}}Y_{l_{i}'0}(\widehat{\mathbf{v}})_{2}F_{1}(n_{i2},i\nu_{t}+l_{i}'+\omega_{i}+\delta_{i},l_{i}'+\omega_{i}+\delta_{i}+1,\tau'/a_{+}), \qquad (57)$$

$$M_{3} = 2a_{+}^{-1} (-2\rho)^{\omega_{i}} (a_{0}\sigma)^{\delta_{i}} v_{i_{i}}^{l'} Y_{l_{i}^{\prime}0}(\hat{\mathbf{v}})(n_{i2})(i\nu_{i} + l_{i}^{\prime} + \omega_{i} + \delta_{i})$$

$$\times {}_{2}F_{1}(n_{i2} + 1, i\nu_{i} + l_{i}^{\prime} + \omega_{i} + \delta_{i} + 1, l_{i}^{\prime} + \omega_{i} + \delta_{i} + 2, \tau^{\prime}/a_{+})/(l_{i}^{\prime} + \omega_{i} + \delta_{i} + 1),$$
(58)

$$M = (-2\alpha)^{\omega_i} (q, \alpha)^{\delta_i} C (m'-1) u^{l'_i-1} \cdot E (n+i) u^{l'_i+1} + \omega_i + \delta_i l' + \omega_i + \delta_i + 1 \sigma'_i (q, -)$$
(59)

$$M_{4} = (-2\rho)^{\omega_{i}} (a_{0}\sigma)^{\delta_{i}} C_{1}(m_{i}=1)^{\omega_{i}} 2r_{1}(n_{i2}, lv_{l}+l_{i}+\omega_{i}+\delta_{i}, l_{i}+\omega_{i}+\delta_{i}+1, r'/a_{+}),$$
(39)
$$M_{4} = (-2\rho)^{\omega_{i}} (a_{0}\sigma)^{\delta_{i}} C_{1}(m_{i}=1)^{\omega_{i}} C_{1}(m_{i}=1)^{\omega_{i}}$$

$$M_{5} = (-2\rho)^{-1} (a_{0}\sigma)^{-1} v^{-1} C_{3}(m_{i}=0) {}_{2}F_{1}(n_{i}, v_{t}+v_{i}+\omega_{i}+\sigma_{i}, v_{i}+\omega_{i}+\sigma_{i}+1, \tau/a_{+}),$$
(60)

$$M_{6} = (-2\rho)^{\omega_{i}} (a_{0}\sigma)^{\sigma_{i}} v^{\iota_{i}-2} C_{2}(m_{i}'=0) {}_{2}F_{1}(n_{i2}, i\nu_{t}+l_{i}'+\omega_{i}+\delta_{i}, l_{i}'+\omega_{i}+\delta_{i}+1, \tau'/a_{+}),$$

$$(61)$$

$$C_{1}(m_{i}') = N_{yl_{i}'m_{i}'} \sum_{\mathbf{K}=0}^{|\mathbf{K}_{i}| \cdots |\mathbf{K}_{i}|} (-1)^{\mathbf{K}} \frac{(2l_{i}-2\mathbf{K})!}{2^{l_{i}'}(l_{i}'-\mathbf{K})!(l_{i}'-m_{i}'-2\mathbf{k})!\mathbf{K}!},$$
(62)

$$N_{yl'_{i}m'_{i}} = \epsilon \left[\frac{(2l'_{i}+1)(l'_{i}-|m'_{i}|)!}{4\pi(l'_{i}+|m'_{i}|)!} \right]^{1/2},$$
(63)

with $\epsilon = (-1)^{m'_i}$ for $m'_i > 0$ and $\epsilon = 1$ for $m'_i \le 0$,

$$C_{2}(m_{i}') = N_{yl_{i}'m_{i}'} \sum_{\mathbf{K}=0}^{\left[(l_{i}'-m_{i}')/2\right]} (-1)^{\mathbf{K}} \frac{(2l_{i}'-2\mathbf{K})!2\mathbf{K}}{2^{l_{i}'}(l_{i}'-\mathbf{K})!(l_{i}'-m_{i}'-2\mathbf{K})!\mathbf{K}!},$$
(64)

$$C_{3}(m_{i}') = N_{yl_{i}'m_{i}'} \sum_{\mathbf{K}=0}^{[(l_{i}'-m_{i}')/2]} (-1)^{\mathbf{K}} \frac{(2l_{i}'-2\mathbf{K})!(l_{i}'-2\mathbf{K})}{2^{l_{i}'}(l_{i}'-\mathbf{K})!(l_{i}'-m_{i}'-2\mathbf{K})!\mathbf{K}!},$$
(65)

 $\hat{i},\,\hat{j},\,and\,\hat{k}$ being the three unit vectors in a Cartesian coordinate system.

C. Evaluation of the integrals J_1 and K

The J_1 and K integrals in Eqs. (11) and (4) can be written as

$$\mathbf{J}_{1} = \lim_{\epsilon \to 0} i\mathbf{p}' \left[-\frac{\delta}{\delta\epsilon} \right] \int d\mathbf{x} \frac{\exp(-i\mathbf{p}' \cdot \mathbf{x} - \epsilon x)}{x} \Phi_{n_{i}l_{i}m_{i}}(\mathbf{x}) {}_{1}F_{1}(i\nu_{i}; 1; i\nu x + i\mathbf{v} \cdot \mathbf{x}) , \qquad (66)$$

$$\mathbf{K} = v \nabla_{v} \int d\mathbf{s} \frac{\exp(i\mathbf{q} \cdot \mathbf{s})}{s} \Phi_{n_{f}l_{f}m_{f}}^{*}(\mathbf{s}) {}_{1}F_{1}(iv_{p}; 1; ivs + i\mathbf{v} \cdot \mathbf{s}) .$$
(67)

1659

The evaluation of these integrals (66) and (67) are similar to that of J_2 and need not be repeated here.

III. NUMERICAL RESULTS AND DISCUSSIONS

Calculations have been carried out at incident energies between 10 and 40 MeV for capture into all final states with $n \le 6$ for the N⁷ + H(1s) collision. The calculated total cross sections are displayed and compared with the existing theoretical results.

In support of the present calculations we have calculated the J and K integrals in Eqs. (3) and (4) for a few lowlying bound states and compared the present computed results with those obtained with the help of the parametric differentiation technique. Identical calculations were found in both the methods for some particular values of the input parameter. We have also reproduced the CDW results of Belkić et al.²⁷ for the $H^+ + \hat{H}(1s)$ collision.

In Table I we present our results for the capture cross sections $Q(n) = \sum_{l_m} Q_{nlm}$, into each complete shell as well as the individual cross sections in each sublevel $Q_{nl} = \sum_{m} Q_{nlm}$ for the collisions of fully stripped nitrogen with atomic hydrogen. In order to compare our calculated results with the existing observed results for the total cross section $Q(tot) = \sum_{n} Q(n)$, we calculate them for each individual energy by assuming the cross section Q(n) to be proportional to n^{-3} for $n \ge 7$ and present them in the same table.

In Fig. 1 we compare our results for the $N^{7+} + H(1s)$ collisions with the available eikonal results. It has been explicitly clear from the figure that the eikonal cross sections overestimate the present CDWA calculations throughout the energy region considered. Unfortunately, experimental results are not available in the highenergy region to compare the present theoretical values. The only experimental value of Goffe et al.¹² at 170 KeV/amu (not shown in the figure) underestimates the present calculated cross section. The discrepancy may be attributed to the fact that the CDW approximation is essentially a high-energy approximation and is not expected to be valid at this energy value. We have also observed that the total capture cross sections obtained with $n \le 6$ and $n \le 5$ differ to the extent of 13% at 10 MeV, below 2% at 20 MeV, and less than 1% at 40 MeV in nitrogen. At 10 MeV the maximum contribution to the total capture cross section comes from the state with n = 3. The population of cross section is maximum with n = 2 at 20 MeV and at 40 MeV the ground-state capture is dominant. This is attributed to the fact that at high energy the capture probability is maximum at small values of input parameter and, consequently, the electron transfer into the inner shells is more dominant.

The *l*-dependent cross sections Q_{nl} indicate a maximum at l = n - 1 for n = 2 at 10 and 20 MeV. It has been observed from Table I that at the higher energy, the distributions are strongly affected by the momentum-transfer effects and the cross sections are gradually reduced with the increase of l. A similar trend has also been observed in the earlier calculations.^{17,24,28} Although we have not shown the *m*-dependent cross sections in the present table, it has also been found that the distributions over m

Projectile energy E (MeV) Q_{1s} $Q_{(1)}$ Q_{2s} Q_{2p} Q_{2p} $Q_{(2)}$ Q_{3s} Q_{3p} Q_{3p} Q_{3d} $Q_{(3)}$ Q_{4s} Q_{4p} energy E (MeV) Q_{1s} Q_{1s} Q_{1s} Q_{1s} Q_{2s} Q_{3p} Q_{3s} Q_{3p} Q_{3d} Q_{3} Q_{4s} Q_{4p}	-
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$Q(3)$ Q_{4s} Q_{4p} Q_{4d} Q_{4f} $Q(4)$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1.15[-3] $5.09[-5]$ $3.19[-4]$ $3.52[-4]$ $1.21[-4]$ $8.44[-4]$
40 $2.56[-6]$ $2.56[-6]$ $1.14[-6]$ $1.36[-6]$ $2.50[-6]$ $4.56[-7]$ $5.90[-7]$ $1.64[-7]$ $1.21[-6]$ $2.14[-7]$ $2.85[-7]$ Q_{55} Q_{5p} Q_{5d} Q_{5f} Q_{5f} Q_{50} Q_{6b} Q_{6d} $Q^{a}(6)$ 10 $3.12[-5]$ $1.94[-4]$ $2.25[-4]$ $1.02[-4]$ $4.88[-5]$ $6.00[-4]$ $2.00[-5]$ $1.23[-4]$ $1.46[-5]$ $1.58[-4]$ 20 $7.70[-6]$ $6.99[-6]$ $4.43[-6]$ $1.30[-6]$ $8.26[-7]$ $1.67[-5]$ $1.65[-6]$ $4.77[-6]$ $2.87[-6]$ $8.75[-6]$	3.40[-5] $4.78[-6]$ $1.23[-5]$ $7.19[-6]$ $1.56[-6]$ $2.59[-5]$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1.21[-6] 2.14[-7] 2.85[-7] 1.03[-7] 2.14[-8] 6.23[-7]
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$Q_{bd} = Q^{a}(6) = Q^{b}(ext{tot})$
$20 2 \ 20[-6] 6 \ 99[-6] 4 \ 43[-6] 1 \ 30[-6] 8 \ 26[-7] 1 \ 62[-5] 1 \ 62[-6] 4 \ 27[-6] 8 \ 75[-6] 5 \ 75[-6] 7 \ 7 \ 75[-6] 7 \ 75[-6] 7 \ 75[-6] 7 \ 75[-6] 7 \ 75[-6] \ 7 \ 75[-6] \ 7 \ 75[-6] \ 7 \ 75[$	1.46[-5] $1.58[-4]$ $4.20[-3]$
$\begin{bmatrix} a \\ a \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} a $	2.82[-6] 8.75[-6] 1.92[-4]
$40 \qquad 1.15[-7] 1.55[-7] 6.19[-8] 1.77[-8] 1.57[-8] 3.66[-7] 6.87[-8] 9.29[-8] 3.88[-8] 2.00[-7] 9.10[-7] 1.10$	3.88[-8] $2.00[-7]$ $7.97[-6]$



FIG. 1. Total capture cross sections Q(tot) for the projectile N^{7+} ion incident on ground-state atomic hydrogen. Theory: _____, present work; _____, eikonal calculation (Ref. 20).

for given l and n indicate a maximum at m=0 in the intermediate- and high-energy region. This behavior is also in conformity with the previous calculations.^{44,45} The high probabilities of electron transfer into the m=0 state corresponds to the classical picture that the electron is mostly captured into the orbitals on the collision plane. We have further observed that with the increase of the incident projectile energy, the calculated results for the total

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capture cross sections are found to be uniformly decreasing and the electron transfer into the inner shells becomes more and more dominant.

IV. CONCLUSION

The present method provides an approach to electron capture from an initial arbitrary $n_i l_i m_i$ shell of a hydrogenic target into the final arbitrary $n_f l_f m_f$ shell of the bare projectile in the framework of the CDW approximation. It may be pointed out that all results already calculated in CDW approximations may be generated from this approach as special cases. The method allows for convenient numerical computations of charge transfer cross sections into arbitrary n, l, and m states of the fast, heavy fully stripped projectiles from the ground state of atomic hydrogen. Unfortunately, no experimental results in the high-energy range are available to compare the present calculated results. Detailed experimental investigations would, therefore, be of great help to test the accuracy and reliability of the CDW approximation.

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