Calculation of cross sections for electron capture by fast Li^{3+} ions from atomic hydrogen in the continuum distorted-wave approximation

Shyamal Datta, C. R. Mandal, S. C. Mukherjee, and N. C. Sil
Department of Theoretical Physics, Indian Association for the Cultivation of Science, Jadavpur, Calcutta 700032, India
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A method for the calculation of cross sections for electron capture into arbitrary n, l, and m states of fast bare projectiles in collisions with fully stripped ions and ground-state hydrogenic targets has been proposed in the framework of the continuum distorted-wave approximation. The charge-exchange amplitude has been reduced to a one-dimensional integral in real space which is very convenient for numerical evaluation. The present method is applied in Li^{3+}-H(1s) collisions and the calculated cross sections are in excellent agreement with the experimental data for the incident energies $E \geq 700$ keV.

I. INTRODUCTION

The study of charge-transfer processes between fully or partially stripped ions with atomic hydrogen has recently attracted a great deal of attention both theoretically as well as experimentally in connection with fusion research.[1] The reactions for the above processes are of the form

$$X^{Z_P+} + \mathrm{H}(1s) \rightarrow X^{(Z_P-1)+} + \mathrm{H}^+ , \quad (1)$$

where X^{Z_P+} represents the incident ion. If the incident ion is fully stripped so that Z_P is equal to the nuclear charge, the ion $X^{(Z_P-1)+}$ is hydrogenic and characterized by a set of single-electron quantum numbers nlm. Electron capture from a hydrogen atom by a highly stripped impurity ion in a confined plasma can reduce the penetration of the energetic neutral hydrogen beam which is injected to heat the plasma. Thus the cross sections for electron capture from hydrogen atoms by highly stripped ions of carbon, oxygen, silicon, molybdenum, etc., which are present in tokamak plasmas, are considered to be one of the rate-determining processes in plasma heating. Experimental investigations to determine the charge-transfer cross sections between fully or partially stripped ions with atomic hydrogen have recently been reported by several workers.[2–17]

Previously the theoretical investigations on charge-transfer processes were mainly confined to the calculation of cross sections involving collisions of atoms with protons and alpha particles. But recently, with the advent of multiply charged ion sources, theoretical interest has been focused on the investigation of multicharged ion-atom collisions. However, quantal calculations suffer from serious computational difficulties because with the increase of the projectile charge, the electrons are captured into increasingly higher principal shells of the projectile. For this reason, few theoretical studies have been made of capture into multiply charged heavier ions in the quantum-mechanical approach.

On the other hand, some classical and semiclassical approaches have recently been suggested to get an estimate of the capture cross sections for the heavy stripped ion-atom collisions. Using the Landau-Zener model, Salop and Olson[18] first calculated theoretically the cross sections for charge transfer between the ground-state atomic hydrogen and stripped ions of C, N, O, Ne, Si, and Ar. When the velocity of the incident ion is small compared to the orbital velocity of the bound electron of the target, the wave functions for the system can be conveniently represented in terms of combination of molecular orbitals. In this velocity region Vaaben and Briggs[19] have obtained charge-transfer cross sections for C^{6+}-H collision using an eleven-molecular-state expansion. Harel and Salin[20] have performed three molecular-state calculations for Be^{4+}-H and O^{8+}-H collision cases, whereas Salop and Olson[21] performed a six-molecular-state calculation to determine the charge transfer in C^{6+}-H collision. Olson and Salop[22] also applied a classical trajectory Monte Carlo method to calculate the charge-transfer cross sections between the ground-state atomic hydrogen and some fully and partially stripped ions. At higher velocities it is more appropriate to use approximations based on truncated two-center atomic expansions[23,24] and these are quite convenient over a range of laboratory energies $5-200$ keV amu^{-1} for an incident proton or an alpha particle in which case the number of channels to be considered is small. As the charge of the incident projectile increases, the number of states that give significant contribution in the cross sections become large and it is quite difficult to include all the states of importance in the coupled-channel calculation.

Ryufuku and Watanabe[25] have recently developed the unitarized distorted-wave approximation (UDWA) and absorption-model calculation to study the capture cross sections for collisions of fully stripped projectiles such as H^+, He^{2+}, Li^{3+}, Be^{4+}, B^{5+}, and O^{8+} with atomic hydrogen. For the UDWA all the interactions among the product channels are ignored and the matrix elements are treated as in the case of resonant charge transfer, whereas in the absorption model the product channels are considered to be closely coupled and the transferred electron is assumed not to be recaptured by the hydrogen ion. In the low-energy region Bottcher[26] has attempted the same problem by employing the impact-parameter treatment using a model in which the curve crossings involving an initial state and a number of diabatic states are considered. Bottcher[26] simplified the calculation by considering stationary atomic states in the S matrix instead of the moving atomic states used by Ryufuku and Watanabe.[25]

The prospect of application of the close-coupling method to highly charged ion-atom collisions in the intermediate- and high-energy region is not very hopeful due to the increasing number of open channels, so one is prone to seek a two-state approximation that could be able to yield, with moderate computational effort, reasonably good results in the aforesaid energy region. The two-state atomic-expansion method of Bates[27] have recently been applied by Bransden *et al.*,[28] to calculate the cross sections for capture by He^{2+}, Li^{3+}, Be^{4+}, and B^{5+} ions from atomic hydrogen over the range of incident laboratory energies of $5-200$ keV amu^{-1}. These authors have developed a standard computer package to obtain the overlap and exchange matrix elements for any arbitrary values of n, l, and m using a method proposed by Sin Fai Lam.[29] Their calculated cross sections agree rather well in shape with the experimental data, but always overestimate the experimental findings[6,14] throughout the energy range of the projectiles considered. Datta and Mukherjee[30] have applied the Coulomb-Born (CB) approximation to obtain the charge-transfer cross sections from the ground state of atomic hydrogen by the fully stripped helium-ion impact and in the intermediate- and high-energy region their results show quite good agreement with the experimental results. Using the same approximation, Mandal *et al.*[31] have recently made a theoretical investigation on Li^{3+}-H collision system which takes into account the effect of the Coulomb repulsion between the proton and the positively charged Li^{2+} ion left in the final state, after the completely stripped lithium ion has captured the electron from the target hydrogen atom. The cross sections obtained by the CB approximation are found to be in excellent agreement with the experimental results[6] throughout the energy region considered except at the low-energy region ($E < 275$ keV). The calculated values of the capture cross sections reported by different authors[22,25,28] except Mandal *et al.*[31] are found to overestimate the experimental findings in the intermediate- and high-energy region. Some new theoretical results may perhaps prove worthwhile in clarifying the situation and the present work is an attempt towards this direction.

It has become increasingly apparent that the first-order methods may be inadequate in dealing with electron-capture processes and it is now well established[32–34] that one should take account of the second-order terms to obtain the correct high-energy behavior of charge-transfer cross sections. Halpern and Law[35] have pointed out that the method due to Jackson and Schiff[36] yields unphysical results for highly stripped ions, although it leads to reasonable results for H^+-H collisions. Various types of second-order methods such as the impulse approximation,[37–40] the continuun-intermediate state[41] (CIS), and the continuum-distorted-wave[42] (CDW) method have been proposed in connection with the calculations of charge-transfer cross sections in the high-energy region. In the CDW approximation, first introduced by Cheshire,[42] the associated amplitude for electron capture contains transitions into and from the intermediate states of the continuum. The ambiguity concerning the part played by the internuclear potential is avoided as no term containing the internuclear interaction $V(R)$ occurs through the perturbing potential. On the other hand, correct boundary conditions for the charge-exchange problem are preserved by taking into account the distortion of the wave function due to the internuclear Coulomb potential. The energy dependence of the capture cross sections in the high-energy limit are in agreement with that predicted by the second-Born approximation.[43] A full quantal version of this approximation is given by Gayet,[44] where it is shown that the CDW approximation is obtained as the rigorous first-order term of a perturbation series.[45]

For charge-exchange reactions such as H^+-H, H^+-He, and He^{2+}-H, the CDW method is in excellent agreement[46–48] with experiment in the energy range $E \geq 100$ keV. It is well known that the excitation and the ionization processes dominate over the charge exchange at high-impact energies. Since all channels are open, the final state of the system can be reached in many ways through different elastic, inelastic, or breakup intermediate channels. Owing to the above-mentioned relative importance of inelastic processes, it is expected that the inclusion of intermediate channels describing the excitation or the ionization of two-body subsystems can considerably influence the charge transfer at high energies. The continuum intermediate states are properly taken into account in the CDW approximation and since the CDW method allows for the distortion of the bound electrons by the incident and scattered ion, it is expected to give reliable results in the calculation of the cross sections involving collisions of highly charged ions with atomic targets. Although an extensive study has been performed for collisions of lighter ions with atomic targets, not many detailed calculations have so far been reported for heavy stripped ion-atom collisions using the second-order approximations. Belkić *et al.*[49] have recently calculated the charge-transfer cross sections in the ground state and 2*s*, 2*p*, 3*s*, and 3*p* excited states for Li^{3+}-H collision system and gave an estimate for the total-capture cross sections assuming the validity of the n^{-3} law from $n \geq 4$ level. Capture into the 3*d* state of Li^{2+} ion is also quite important since the third-energy level of Li^{2+} ion is in resonance with H (1*s*). Belkić *et al.* have, however, ignored the contribution of capture into the 3*d* state of Li^{2+} ion in their calculation for the total-capture cross sections. Further, in their calculation for the capture cross sections of the higher excited states, they have used the repeated parametric differentiation technique with respect to suitable parameters.

As the charge of the incident projectile increases, capture cross sections will dominate from higher values of the principal quantum number n of the captured states. The customary procedure for the calculation of cross sections for such high quantum states involves the process of repeated parametric differentiation of the relevant generating function. The number of such differentiations increases with increasing values of n and l. The generation of higher excited states by this procedure makes the problem almost untenable. An alternative procedure which avoids the use of the successive parametric-differentiation technique is necessary to deal with the calculation of cross sections for capture into arbitrary n, l, and m states of the projectile. The present paper is aimed at developing a method for the calculation of cross sections for capture into an arbitrary n l, and m states of fast projectiles in collision with a fully stripped ion and a ground-state hydrogenic target in the framework of the CDW approximation. The present method reduces the scattering amplitude to a one-dimensional integral in real space which is convenient for numerical evaluation. Our proposed approach is quite straightforward and rather simple in the sense that one can easily obtain all the cross sections from a single computer program. This enables one to make a comparative study of the dependence of charge-transfer cross sections on the quantum numbers n, l, m and also on the projectile charge. This method has been applied to calculate the charge-transfer cross sections for the $^7Li^{3+}$-H collision system and the results obtained are compared with the previously reported theoretical results[22,25,28,31] and the existing experimental observations.[6]

In Sec. II the formulation based on the CDW approximation is reviewed.[49] Our method for the evaluation of the scattering amplitude is described in Secs. III, IV, and V. In Sec. VI the numerical results for the cross sections are presented and discussed. Finally, in Sec. VII, a concluding summary of the paper is given. Atomic units are used throughout the paper, unless otherwise stated.

II. FORMULATION OF THE CDW APPROXIMATION

Let $\vec{r}_t$, $\vec{r}_e$, and $\vec{r}_p$ be the respective position vectors of the target nucleus, electron and incident projectile for the process (1) in an arbitrary Galilean frame. We introduce the coordinates

$$\vec{x}=\vec{r}_e-\vec{r}_t \; ,$$
$$\vec{s}=\vec{r}_e-\vec{r}_P \; , \quad (2)$$
$$\vec{R}=\vec{r}_P-\vec{r}_t \; .$$

Let $\vec{r}_\alpha$ be the position vector of the projectile relative to the center-of-mass of the target, while $\vec{r}_\beta$ is a similar vector with the target nucleus and the projectile interchanged. They may be written as

$$\vec{r}_\alpha=\vec{r}_P-\frac{M_t\vec{r}_t+M_e\vec{r}_e}{M_t+M_e} \; ,$$
$$\vec{r}_\beta=\vec{r}_t-\frac{M_P\vec{r}_P+M_e\vec{r}_e}{M_P+M_e} \; , \quad (3)$$

where M_t, M_e, and M_P are, respectively, the masses of the target nucleus, electron, and projectile. Gayet[44] has shown that, in the limit $M_e/\mu \to 0$, where μ is the reduced mass of the whole system, the CDW approximation can be obtained in the series expansion of Dodd and Greider.[45] The "post" form of the transition amplitude in the wave formalism of Dodd and Greider[45] may be expressed as

$$T_{ij}^{\alpha\beta+}=\langle \Phi_j^{\beta-} \mid \omega_\beta^-(v_\beta-W_\beta)[1+g_x^+(v_\alpha-W_\alpha)\omega_\alpha^+ \mid \Phi_i^{\alpha+}\rangle \; . \quad (4)$$

An analogous expression for the "prior" form of the transition amplitude is given by

$$T_{ij}^{\alpha\beta-}=\langle \Phi_j^{\beta-} \mid \omega_\beta^{-*}[1+g_x^+(v_\beta-W_\beta)]^*(v_\alpha-W_\alpha)\omega_\alpha^+ \mid \Phi_i^{\alpha+}\rangle \; , \quad (5)$$

where

$$v_\alpha=-\frac{Z_P}{s}+\frac{Z_PZ_t}{R} \; ,$$
$$v_\beta=-\frac{Z_t}{x}+\frac{Z_PZ_t}{R} \; ,$$
$$W_\alpha=w_\alpha+W_{\alpha d} \; , \quad (6)$$
$$W_\beta=w_\beta+W_{\beta d} \; ,$$
$$g_x^+=(E-H+v_x+i\epsilon)^{-1} \; .$$

w_α, w_β are the distorting potentials which depend only on $\vec{r}_\alpha$ and $\vec{r}_\beta$, and $W_{\alpha d}$ and $W_{\beta d}$ are the Coulomb distorting potentials such that $\Phi_i^{\alpha+}$ and $\Phi_j^{\beta-}$ contain the correct asymptotic Coulomb phases due to the Coulomb interaction between aggregates in the entrance and exit channels, respectively, and v_x is the potential corresponding to a virtual intermediate channel x. The asymptotic states are defined as the solutions of the following equations:

$$(H_{\alpha d}-E)\mid \Phi_i^{\alpha+}\rangle=(H_\alpha+W_{\alpha d}-E)\mid \Phi_i^{\alpha+}\rangle=0 \; , \quad (7)$$

$$(H_{\beta d}-E)\mid \Phi_j^{\beta-}\rangle=(H_\beta+W_{\beta d}-E)\mid \Phi_j^{\beta-}\rangle=0 \; , \quad (8)$$

where

$$H_{\alpha d}=H_\alpha+W_{\alpha d}$$

and

$$H_{\beta d}=H_\beta+W_{\beta d} \; . \quad (9)$$

H_α and H_β are the Hamiltonians for the entrance and the exit channels, respectively. The operators ω_α^+ and ω_β^- are defined by

$$\omega_\alpha^+=1+(E-H_{\alpha d}-w_\alpha+i\epsilon)^{-1}w_\alpha \; ,$$
$$\omega_\beta^-=1+(E-H_{\beta d}-w_\beta-i\epsilon)^{-1}w_\beta \; . \quad (10)$$

H and E are, respectively, the complete Hamiltonian and the total energy of the whole system. In order to calculate $T_{ij}^{\alpha\beta+}$ given by expression (4), let us set

$$\mid \chi_i^{\alpha+}\rangle=\omega_\alpha^+\mid \Phi_i^{\alpha+}\rangle=\mid \Phi_i^\alpha(\vec{x})f(\vec{r}_\alpha)\rangle \; , \quad (11)$$

which has the same asymptotic behavior as $\mid \Phi_i^{\alpha+}\rangle$. We require in Eq. (4) the function

$$\mid \xi_i^{\alpha+}\rangle=[1+g_x^+(v_\alpha-W_\alpha)]\mid \chi_i^{\alpha+}\rangle \; , \quad (12)$$

which in the limit $\epsilon \to 0^+$ satisfies the following equation:

$$(E-H+v_x)\mid \xi_i^{\alpha+}\rangle=0 \; , \quad (13)$$

provided that

$$v_x\mid \chi_i^{\alpha+}\rangle=0 \; . \quad (14)$$

The solution of equation (13) may be written in the form

$$\mid \xi_i^{\alpha+}\rangle=\mid \Phi_i^\alpha(\vec{x})h^+\rangle \; , \quad (15)$$

such that

$$\xi_i^{\alpha +} \underset{r_\alpha \to \infty}{\longrightarrow} \Phi_i^\alpha(\vec{x})\exp\left[i\vec{k}_\alpha\cdot\vec{r}_\alpha + i\frac{Z_P(Z_t-1)}{v}\ln(k_\alpha r_\alpha - \vec{k}_\alpha\cdot\vec{r}_\alpha)\right] . \tag{16}$$

Equation (13) may be written as

$$\Phi_i^\alpha(\vec{x})(E-\epsilon_i - H_0 - v_\alpha)h^+ + \frac{1}{a}\vec{\nabla}_x\Phi_i^\alpha(\vec{x})\cdot\vec{\nabla}_x h^+ + v_x\xi_i^{\alpha+} = 0 , \tag{17}$$

ϵ_i being the energy of target atom, where

$$H_0 = -\frac{1}{2\mu_\alpha}\nabla_{r_\alpha}^2 - \frac{1}{2a}\nabla_x^2 = -\frac{1}{2\mu_\beta}\nabla_{r_\beta}^2 - \frac{1}{2b}\nabla_s^2 , \qquad a = M_e M_t/(M_e+M_t) , \qquad b = M_e M_P/(M_e+M_P) . \tag{18}$$

μ_α and μ_β are the reduced masses in the initial and final channels, respectively. Instead of choosing for v_x a local two-body potential, Gayet[44] takes v_x as an operator such that applied to an arbitrary function Ψ of $\vec{x}$ and $\vec{r}_\alpha$ (or $\vec{s}$ and $\vec{r}_\beta$), the following relationship holds:

$$v_x\Psi = -\frac{1}{a}\vec{\nabla}_x\Phi_i^\alpha(\vec{x})\cdot\vec{\nabla}_x[\Psi/\Phi_i^\alpha(\vec{x})] . \tag{19}$$

Equation (17) becomes separable in the variables $\vec{s}$ and $\vec{r}_\beta$ if $\vec{R}$ is replaced by $-\vec{r}_\beta$, which is justified in the limit $M_{P,t} \gg M_e$. The solution of h^+ becomes[49]

$$h^+ = \mu^{-i\nu_P} N(\nu_P)N(\nu)\exp(i\vec{k}_\alpha\cdot\vec{r}_\alpha)\,{}_1F_1(i\nu_P;1;ivs + i\vec{v}\cdot\vec{s})\,{}_1F_1(-i\nu;1;ik_\alpha r_\beta + i\vec{k}_\alpha\cdot\vec{r}_\beta) , \tag{20}$$

where

$$\begin{aligned} N(\nu_P) &= \Gamma(1-i\nu_P)\exp(\pi\nu_P/2) , \\ N(\nu) &= \Gamma(1+i\nu)\exp(\pi\nu/2) , \\ \nu_P &= Z_P/v , \\ \nu &= Z_P Z_t/v , \\ v &= k_\alpha/\mu . \end{aligned} \tag{21}$$

$\vec{k}_\alpha$ is the momentum of the projectile in the initial channel. The state vector in the exit channel is given by:

$$|\chi_j^{\beta-}\rangle = \omega_\beta^- |\Phi_j^{\beta-}\rangle . \tag{22}$$

We require $|\chi_j^{\beta-}\rangle$ as:

$$|\chi_j^{\beta-}\rangle = |\Phi_j^{\beta-}(\vec{s})h^-\rangle , \tag{23}$$

where h^- is chosen to be a continuum wave. In the limit $\epsilon \to 0^+$, $|\chi_j^{\beta-}\rangle$ satisfies the equation:

$$(E - H + v_\beta - W_\beta)|\chi_j^{\beta-}\rangle = 0 \tag{24}$$

with the appropriate boundary condition:

$$\chi_j^{\beta-} \underset{r_\beta \to \infty}{\longrightarrow} \Phi_j^\beta(\vec{s})\exp\left[-i\vec{k}_\beta\cdot\vec{r}_\beta - i\frac{Z_t(Z_P-1)}{v'}\ln(k_\beta r_\beta - \vec{k}_\beta\cdot\vec{r}_\beta)\right] . \tag{25}$$

Equation (24) reduces to

$$(E-\epsilon_j - H_0 - v_\beta)h^- + \frac{1}{b}\vec{\nabla}_s\Phi_j^\beta(\vec{s})\cdot\vec{\nabla}_s h^- + U_\beta[\Phi_j^\beta(\vec{s})h^-] = 0 , \tag{26}$$

where $U_\beta = v_\beta - W_\beta$ and ϵ_j is the energy of the final bound state. Choosing U_β as an operator analogous to $v_x\Psi$ such that

$$U_\beta\Psi=-\frac{1}{b}\vec{\nabla}_s\Phi_j^\beta(\vec{s})\cdot\vec{\nabla}_s[\Psi/\Phi_j^\beta(\vec{s})]\ , \tag{27}$$

the solution of Eq. (26), in the limit $M_{P,t}\gg M_e$ becomes[49]

$$h^-=\mu^{i\nu_t}N^*(\nu_t)N^*(\nu')\exp(-i\vec{k}_\beta\cdot\vec{r}_\beta)\,{}_1F_1(-i\nu_t;1;-iv'x-i\vec{v}\,'\cdot\vec{x})\,{}_1F_1(i\nu';1;-ik_\beta r_\alpha-i\vec{k}_\beta\cdot\vec{r}_\alpha)\ , \tag{28}$$

where

$$\begin{aligned}\nu_t&=Z_t/v'\ ,\\ \nu'&=Z_PZ_t/v'\ ,\\ v'&=k_\beta/\mu\ .\end{aligned} \tag{29}$$

$\vec{k}_\beta$ is the momentum of the scattered particle in the final channel. In the limit $M_{P,t}\gg M_e$, the "post" form of transition amplitude becomes

$$T_{ij}^{\alpha\beta+}=-\int d\vec{r}_\beta d\vec{s}\ \Phi_i^\alpha(\vec{x})h^+\vec{\nabla}_s\Phi_j^{\beta*}(\vec{s})\cdot\vec{\nabla}_s h^{-*}\ . \tag{30}$$

An analogous expression may be derived for the "prior" form of the transition amplitude:

$$T_{ij}^{\alpha\beta-}=-\int d\vec{r}_\alpha d\vec{x}\ \Phi_j^{\beta*}(\vec{s})h^{-*}\vec{\nabla}_x\Phi_i^\alpha(\vec{x})\cdot\vec{\nabla}_s h^+\ . \tag{31}$$

The expressions of $T_{ij}^{\alpha\beta\pm}$ in (30) and (31) may be reduced to that given by the continuum distorted wave of Cheshire[42] when one replaces the product

$$[N(\nu)]^2\,{}_1F_1(-i\nu;1;ik_\alpha r_\beta+i\vec{k}_\alpha\cdot\vec{r}_\beta)\,{}_1F_1(-i\nu;1;ik_\beta r_\alpha+i\vec{k}_\beta\cdot\vec{r}_\alpha)\ , \tag{32}$$

by its asymptotic limit when $M_{P,t}\to\infty$. Introducing the usual vectors $\vec{\eta}$ and $\vec{\rho}$ such that

$$\begin{aligned}&\vec{R}=\vec{\rho}+\vec{Z}\ ,\\ &\vec{k}_\beta-\vec{k}_\alpha\simeq\vec{\eta}+\left[\frac{M_e}{2}\frac{(M_t-M_P)}{(M_P+M_t+M_e)}+\frac{\epsilon_i-\epsilon_j}{v^2}\right]\vec{v}\ ,\\ &\vec{\eta}\cdot\vec{v}=\vec{\eta}\cdot\vec{Z}=\vec{\rho}\cdot\vec{v}=\vec{\rho}\cdot\vec{Z}=0\ ,\end{aligned} \tag{33}$$

$\vec{\eta}$ being the component of momentum transfer in the plane perpendicular to $\vec{v}$, Gayet[44] showed that the limit of (32) takes the form $(\mu v\rho)^{2i\nu}$.

Since scattering at small angles contribute to the total cross section, one has $\nu'\approx\nu$. The transition amplitude of the CDW approximation for forward capture is

$$Tij^{\alpha\beta\pm}=\mp N(v)\int d\vec{r}_\beta d\vec{s}\ (\mu v\rho)^{2i\nu}\exp(i\vec{p}\cdot\vec{x}+i\vec{q}\cdot\vec{s})Lij^{\alpha\beta\pm}\ , \tag{34}$$

where

$$\begin{aligned}&N(v)=\Gamma(1-i\nu_t)\Gamma(1-i\nu_P)\exp[\tfrac{1}{2}\pi(\nu_P+\nu_t)]\ ,\\ &\vec{p}=-\vec{\eta}-\left[\frac{\epsilon_i-\epsilon_j}{v^2}+\frac{M_e}{2}\right]\vec{v}\ ,\\ &\vec{q}=\vec{\eta}+\left[\frac{\epsilon_i-\epsilon_j}{v^2}-\frac{M_e}{2}\right]\vec{v}\ ,\\ &L_{ij}^{\alpha\beta+}=\Phi_i^\alpha(\vec{x})\,{}_1F_1(i\nu_p;1;ivs+i\vec{v}\cdot\vec{s})\vec{\nabla}_s\Phi_j^{\beta*}(\vec{s})\vec{\nabla}_x\,{}_1F_1(i\nu_t;1;ivx+i\vec{v}\cdot\vec{x})\ ,\\ &L_{ij}^{\alpha\beta-}=\Phi_j^{\beta*}(\vec{s})\,{}_1F_1(i\nu_t;1;ivx+i\vec{v}\cdot\vec{x})\vec{\nabla}_x\Phi_i^\alpha(\vec{x})\vec{\nabla}_s\,{}_1F_1(i\nu_P;1;ivs+i\vec{v}\cdot\vec{s})\ .\end{aligned} \tag{35}$$

In the present investigation, since we are dealing with exact bound-state wave functions, there arises no post-prior discrepancy. Then neglecting all unimportant phase factors which do not contribute in the total capture cross section, the prior form of transition amplitude becomes

$$T_{ij}^{\alpha\beta-} = -N(v)\vec{J}\cdot\vec{K} \ , \tag{36}$$

where

$$\vec{J} = \int d\vec{x}\, \exp(i\vec{p}\cdot\vec{x})[\vec{\nabla}_x \Phi_i^{\alpha}(\vec{x})]\,{}_1F_1(i\nu_t;1;ivx+i\vec{v}\cdot\vec{x}) \ , \tag{37}$$

$$\vec{K} = \int d\vec{s}\, \exp(i\vec{q}\cdot\vec{s})\Phi_j^{\beta *}(\vec{s})\vec{\nabla}_s\, {}_1F_1(i\nu_P;1;ivs+i\vec{v}\cdot\vec{s}) \ . \tag{38}$$

This form of transition amplitude (36) has also been used by Belkić and McCarroll[50] to investigate the projectile charge dependence of electron-capture cross sections in the CDW approximation. The total-capture cross section is calculated using the relation

$$Q_{ij} = \int \left| \frac{T_{ij}^{\alpha\beta-}(\vec{\eta})}{2\pi v} \right|^2 d\vec{\eta} \ . \tag{39}$$

III. EVALUATION OF THE INTEGRAL $\vec{J}$

The ground-state wave function of the target atom is

$$\Phi_i^{\alpha}(\vec{x}) = \frac{1}{\sqrt{\pi}}(Z_t)^{3/2}\exp(-Z_t x) \ ,$$

Z_t being the nuclear charge of the target. The $\vec{J}$ integral in Eq. (37) can be expressed as

$$\vec{J} = i\left[\frac{Z_t^5}{\pi}\right]^{1/2} \vec{\nabla}_P \int d\vec{x}\, \frac{\exp(i\vec{p}\cdot\vec{x}-Z_t x)}{x}\, {}_1F_1(i\nu_t;1;ivx+i\vec{v}\cdot\vec{x}) \ . \tag{40}$$

We, now use the integral representation[51] of the confluent hypergeometric function

$${}_1F_1(i\alpha;1;z) = \frac{1}{2\pi i}\oint_{\Gamma}^{(0+,1+)} dt\, p'(\alpha,t)\exp(zt) \tag{41}$$

with

$$p'(\alpha,t) = t^{i\alpha-1}(t-1)^{-i\alpha} \ . \tag{42}$$

Γ is a closed contour encircling the two points 0 and 1 once counterclockwise. At the point where the contour crosses the real axis to the right-hand side of 1, $\arg(t)$ and $\arg(t-1)$ are both zero. After proper rearrangement $\vec{J}$ integral becomes

$$\vec{J} = i\left[\frac{Z_t^5}{\pi}\right]^{1/2} \vec{\nabla}_P \frac{1}{2\pi i}\oint_{\Gamma}\int dt\, d\vec{x}\, t^{i\nu_t-1}(t-1)^{-i\nu_t} \frac{\exp[-(Z_t - ivt)x + i(\vec{p}+\vec{v}t)\cdot\vec{x}]}{x} \ . \tag{43}$$

Performing the space integration $\vec{J}$ integral reduces to

$$\vec{J} = 4\pi i\left[\frac{Z_t^5}{\pi}\right]^{1/2} \vec{\nabla}_P \frac{1}{2\pi i} \times \oint_{\Gamma} dt\, t^{i\nu_t-1}(t-1)^{-i\nu_t}\, \frac{1}{A_1 - B_1 t} \tag{44}$$

with

$$A_1 = p^2 + Z_t^2 \ ,$$

$$B_1 = 2iZ_t v - 2\vec{p}\cdot\vec{v} \ . \tag{45}$$

Thus we have

$$\vec{J} = 4\pi i\left[\frac{Z_t^5}{\pi}\right]^{1/2} \vec{\nabla}_P \frac{1}{A_1}\left[1-\frac{B_1}{A_1}\right]^{-i\nu_t} ,$$

$$= 4\pi i\left[\frac{Z_t^5}{\pi}\right]^{1/2} \vec{\nabla}_P \left[\frac{1}{p^2+Z_t^2}\right] \times \left[1+\frac{2(\vec{p}\cdot\vec{v}-iZ_t v)}{(p^2+Z_t^2)}\right]^{-i\nu_t} \ . \tag{46}$$

IV. EVALUATION OF THE INTEGRAL $\vec{K}$

The $\vec{K}$ integral in Eq. (38) may be expressed as

$$\vec{K}=v\vec{\nabla}_v\int d\vec{s}\,\frac{\exp(i\vec{q}\cdot\vec{s})}{s}\Phi_j^{\beta_*}(\vec{s})\times{}_1F_1(i\nu_P;1;ivs+i\vec{v}\cdot\vec{s})\ . \qquad (47)$$

The final bound-state wave function characterized by the set of quantum numbers n, l, and m may be written as

$$\Phi_j^{\beta}(\vec{s})=\Phi_{nlm}(\vec{s})=N_{nlm}R_{nl}(s)Y_{lm}(\hat{s})\ . \qquad (48)$$

N_{nlm} is the normalization constant given by

$$N_{nlm}=-\frac{(2\gamma_n)^{l+1}}{(n+l)!}\left[\frac{\gamma_n(n-l-1)!}{n(n+l)!}\right]^{1/2} \qquad (49)$$

with $\gamma_n=Z_P/n$. $R_{nl}(s)$ is the radial wave function, $Y_{lm}(\hat{s})$ being the spherical harmonics. $R_{nl}(s)$ may be written as

$$R_{nl}(s)=s^l\exp(-\gamma_n s)L_{n+l}^{2l+1}(2\gamma_n s)\ , \qquad (50)$$

where $L_\mu^\nu(x)$ is the associated Laguerre polynomial of degree μ and of order ν. We use the integral representation[51] of the confluent hypergeometric function

$${}_1F_1(i\nu_P;1;t)=\frac{1}{2\pi i}\oint_\Gamma^{(0+,1+)}dz\exp(zt)\times p''(\nu_P,z) \qquad (51)$$

with

$$p''(\nu_P,z)=z^{i\nu_P-1}(z-1)^{-i\nu_P}\ . \qquad (52)$$

Γ is a closed contour encircling the two points 0 and 1 once counterclockwise. Making use of the above relations, we obtain the $\vec{K}$ integral as

$$\vec{K}=N_{nlm}v\vec{\nabla}_v\frac{1}{2\pi i}\oint_\Gamma dz\,p''(\nu_P,z)I\ , \qquad (53)$$

where

$$I=\int d\vec{s}\,\frac{\exp(i\vec{Q}\cdot\vec{s}+ivsz)}{s}R_{nl}(s)Y_{lm}^*(\hat{s})\ , \qquad (54)$$

and

$$\vec{Q}=\vec{q}+\vec{v}z\ . \qquad (55)$$

Following the integral representation[52] of the Laguerre polynomial

$$L_{n+l}^{2l+1}(2\gamma_n s)=-\frac{(n+l)!}{2\pi i}\oint_C\frac{dt\exp[-2\gamma_n st/(1-t)]}{(1-t)^{2l+2}t^{n-l}} \qquad (56)$$

(the contour C encloses the origin), we obtain the integral I in Eq. (54) as

$$I=-(n+l)!\frac{1}{2\pi i}\oint_C\frac{dt}{(1-t)^{2l+2}t^{n-l}}I_1\ , \qquad (57)$$

where

$$I_1=\int d\vec{s}\,\frac{\exp(-\mu s+i\vec{Q}\cdot\vec{s})}{s}s^lY_{lm}^*(\hat{s})\ , \qquad (58)$$

and

$$\mu=\gamma_n\left[\frac{1+t}{1-t}\right]-ivz\ . \qquad (59)$$

To evaluate I_1 we first expand $e^{i\vec{Q}\cdot\vec{s}}$ in terms of the spherical harmonics, i.e.,

$$\exp(i\vec{Q}\cdot\vec{s})=4\pi\sum_{LM}i^Lj_l(Qs)Y_{LM}^*(\hat{Q})Y_{LM}(\hat{s})\ . \qquad (60)$$

Then the integration over the entire solid angle in (58) yields

$$I_1=4\pi i^lY_{lm}^*(\hat{Q})\int_0^\infty J_l(Qs)s^{l+1}\times\exp(-\mu s)ds\ . \qquad (61)$$

Using $j_l(Qs)=\sqrt{\pi/2Qs}\,J_{l+1/2}(Qs)$, the radial integration in (61) can be easily performed using the relation,[53]

$$\int_0^\infty\exp(-\alpha x)J_\nu(\beta x)x^\nu dx=\frac{(2\beta)^\nu\Gamma(\nu+\frac{1}{2})}{\sqrt{\pi}(\alpha^2+\beta^2)^{\nu+1/2}}\ , \qquad (62)$$

$$(\mathrm{Re}\nu>-\tfrac{1}{2}\text{ and }\mathrm{Re}\alpha>|\mathrm{Im}\beta|)\ .$$

The integral I_1 in (61) reduces to

$$I_1=4\pi l!i^lY_{lm}^*(\hat{Q})(2Q)^l/(\mu^2+Q^2)^{l+1}\ . \qquad (63)$$

Putting the result of (63) in (57) we get

$$I=-(n+l)!4\pi l!i^lY_{lm}^*(\hat{Q})(2Q)^l\frac{1}{2\pi i}\times\oint_C\frac{F(t)dt}{t^{n-l}}\ . \qquad (64)$$

The function $F(t)$ is given by

$$F(t)=[A(1-2Bt+Dt^2)]^{-(l+1)} \tag{65}$$

with

$$A=(\gamma_n-ivz)^2+Q^2\ ,$$
$$B=(Q^2-v^2z^2-\gamma_n^2)/A\ , \tag{66}$$
$$D=[(\gamma_n+ivz)^2+Q^2]/A\ .$$

We employ the following expression[54]:

$$(1-2uz+u^2)^{-\nu}=\sum_{\mu=0}^{\infty}C_\mu^\nu(z)u^\mu\ . \tag{67}$$

The coefficients $C_\mu^\nu(z)$ of the above series are the Gegenbauer polynomials of degree μ and of order ν. Thus

$$F(t)=A^{-(l+1)}\sum_{\nu=0}^{\infty}C_\nu^{l+1}(\lambda)(\varphi t)^\nu \tag{68}$$

with

$$\lambda^2=B^2/D \text{ and } \varphi^2=D\ . \tag{69}$$

Substituting (68) in (64) one obtains

$$I=-(n+l)!4\pi l!i^l Y_{lm}^*(\hat{Q})(2Q)^l A^{-(l+1)}\frac{1}{2\pi i}\oint\frac{dt}{t^{n-l}}\sum_{\nu=0}^{\infty}C_\nu^{l+1}(\lambda)(\varphi t)^\nu\ . \tag{70}$$

Since the contour integral is equal to $2\pi i$ times the sum of the residues at the singularities within the contour (here the singularity lies at the origin only), we can easily find the result by collecting the coefficients of t^{-1} from the expansion of the integrand in terms of t. On substitution of the result of contour integration we obtain

$$I=-(n+l)!4\pi l!i^l Y_{lm}^*(\hat{Q})(2Q)^l C_{n-l-1}^{l+1}(\lambda)\Delta\ , \tag{71}$$

where we have put

$$\Delta^2=[(\gamma_n+ivz)^2+Q^2]^{n-l-1}A^{-(n+l+1)}\ . \tag{72}$$

Substituting the value of I given by (71) in Eq. (53) for $\vec{K}$ integral, we get

$$\vec{K}=-(n+l)!4\pi l!i^l N_{nlm}v\vec{\nabla}_v\frac{1}{2\pi i}\oint_\Gamma^{(0+,1+)}dz\,z^{i\nu_P-1}(z-1)^{-i\nu_P}Y_{lm}^*(\hat{Q})(2Q)^l C_{n-l-1}^{l+1}(\lambda)\Delta\ . \tag{73}$$

V. EVALUATION OF THE TRANSITION AMPLITUDE $T_{ij}^{\alpha\beta-}$

After performing the dot product between the two integrals $\vec{J}$ and $\vec{K}$, one obtains the transition amplitude as

$$T_{ij}^{\alpha\beta-}=N(v)N_{JK}\frac{1}{2\pi i}\oint_\Gamma dz\,z^{i\nu_P-1}(z-1)^{-i\nu_P}zf(z)\ , \tag{74}$$

where

$$N_{JK}=(n+l)!4\pi l!(2i)^l N_{nlm}v\ ,$$
$$f(z)=C_1A'v^2-C_2A'\vec{p}\cdot\vec{v}+C_1B'\vec{q}\cdot\vec{v}-C_2B'\vec{p}\cdot\vec{q}+R_3[C_1(v_x-iv_y)-C_2(p_x-ip_y)]\ ,$$
$$A'=a_1R_1+a_1R_2z-a_2S_2+a_3H_1\ ,$$
$$B'=a_1R_2+a_2S_1-a_3D_1\ ,$$
$$a_1=C_{n-l-1}^{l+1}(\lambda)\Delta\ ,$$
$$a_2=Y_{lm}^*(\hat{Q})Q^l\Delta\ ,$$
$$a_3=Y_{lm}^*(\hat{Q})Q^lC_{n-l-1}^{l+1}(\lambda)\ ,$$
$$H_1=P_1'^{(n-l-3)/2}A''^{-(n+l+3)/2}H\ ,$$
$$D_1=P_1'^{(n-l-3)/2}A''^{-(n+l+3)/2}D'\ ,$$

$$A''=(\gamma_n-ivz)^2+Q^2 ,$$
$$P_1'=(\gamma_n+ivz)^2+Q^2 ,$$
$$H=[n(Q^2+\gamma_n^2-v^2z^2)+(l+1)2i\gamma_n vz]\frac{2i\gamma_n}{v} ,$$
$$D'=2[2i\gamma_n vzn+(l+1)(Q^2+\gamma_n^2-v^2z^2)] ,$$
$$S_1=4\gamma_n^2(Q^2+\gamma_n^2+v^2z^2)/(A''P_1')^{3/2}$$
$$S_2=4\gamma_n^2 z(Q^2-\gamma_n^2-v^2z^2)/(A''P_1')^{3/2}$$
$$C_1=8\pi i\left[\frac{Z_t}{\pi}\right]^{1/2}(-i\nu_t)\frac{1}{(p^2+Z_t^2)^2}\left[1+\frac{2(\vec{p}\cdot\vec{v}-iZ_t v)}{(p^2+Z_t^2)}\right]^{-i\nu_t-1} ,$$
$$C_2=4\pi i\left[\frac{Z_t}{\pi}\right]^{1/2}\left[\frac{2}{(p^2+Z_t^2)^2}\left[1+\frac{2(\vec{p}\cdot\vec{v}-iZ_t v)}{(p^2+Z_t^2)}\right]^{-i\nu_t}+(-i\nu_t)\frac{4}{(p^2+Z_t^2)^3}\left[1+\frac{2(\vec{p}\cdot\vec{v}-iZ_t v)}{(p^2+Z_t^2)}\right]^{-i\nu_t-1}(\vec{p}\cdot\vec{v}-iZ_t v)\right] , \quad (75)$$
$$R_1=N_R\frac{1}{2^l v}\sum_{k=0}^{L''}(-1)^k\frac{(2l-2k)!}{(l-k)!(l-m-1-2k)!k!}Q_z^{l-m-1-2k}Q^{2k} ,$$
$$L''=\begin{cases}\frac{1}{2}(l-m-1) & \text{when } (l-m) \text{ is odd} ,\\ \frac{1}{2}(l-m-2) & \text{when } (l-m) \text{ is even} ,\end{cases}$$
$$N_R=(-1)^m\left[\frac{(2l+1)(l-m)!}{4\pi(l+m)!}\right]^{1/2} ,$$
$$R_2=N_R 2^{1-l}\sum_{k=1}^{L'}(-1)^k\frac{(2l-2k)!}{(l-k)!(l-m-2k)!(k-1)!}Q_z^{l-m-2k}Q^{2k-2} ,$$
$$L'=\begin{cases}\frac{1}{2}(l-m) & \text{when } (l-m) \text{ is even} ,\\ \frac{1}{2}(l-m-1) & \text{when } (l-m) \text{ is odd} ,\end{cases}$$
$$R_3=N_R 2^{-l}\sum_{k=0}^{L'''}(-1)^k\frac{(2l-2k)!}{(l-k)!(l-m-2k)!k!}Q_z^{l-m-2k}Q^{2k}(Q_x-iQ_y)^{m-1} ,$$
$$L'''=\begin{cases}\frac{1}{2}(l-m) & \text{when } (l-m) \text{ is even} ,\\ \frac{1}{2}(l-m-1) & \text{when } (l-m) \text{ is odd} .\end{cases}$$

The integral $T_{ij}^{\alpha\beta-}$ in (74) may be equivalently written as

$$T_{ij}^{\alpha\beta-}=\frac{N}{2\pi i}\exp(-\pi\nu_P)\oint_\Gamma dz\, z^{i\nu_P}(1-z)^{-i\nu_P}f(z) , \quad (76)$$

where $N=N(v)N_{JK}$. Γ being a closed contour surrounding the points $z=0$ and $z=1$ once counterclockwise and the lower part of Γ is located on the real axis. We choose this form for convenience of numerical evaluation of the integral. To evaluate this one-dimensional complex integral (76) we adopt the procedure of Mukherjee *et al.*,[55] with some modifications. The function $f(z)$ is free from singularity in the region $0\le z\le 1$. For the evaluation of $T_{ij}^{\alpha\beta-}$ we introduce a function $g(z)=z[f(1)-f(0)]+f(0)$ in the integrand by virtue of which the integrand vanishes at $z=0$ and $z=1$. We may thus write

$$T_{ij}^{\alpha\beta-}=\frac{N}{2\pi i}\exp(-\pi\nu_P)\oint_\Gamma dz\, z^{i\nu_P}(1-z)^{-i\nu_P}[f(z)-g(z)+g(z)] \; . \tag{77}$$

Following Mukherjee *et al.*[55] we convert (77) into a real one-dimensional integral as

$$\begin{aligned} T_{ij}^{\alpha\beta-}=&\frac{N}{2\pi i}[\exp(-\pi\nu_P)-\exp(\pi\nu_P)]\int_0^1 dz\, z^{i\nu_P}(1-z)^{-i\nu_P}F(z)+\frac{N}{2\pi i}\exp(-\pi\nu_P)\\ &\times\oint_\Gamma dz\, z^{i\nu_P+1}(1-z)^{-i\nu_P}[f(1)-f(0)]\\ &+\frac{N}{2\pi i}\exp(-\pi\nu_P)\oint_\Gamma dz\, z^{-i\nu_P}(1-z)^{-i\nu_P}f(0)\; , \end{aligned} \tag{78}$$

where

$$F(z)=f(z)-g(z) \; .$$

Since

$$\frac{\exp(-\pi\nu_P)}{2\pi i}\oint dz\, z^{i\nu_P-1}(1-z)^{-i\nu_P}\exp(zt)={}_1F_1(i\nu_P;1;t)\; , \tag{79}$$

expanding the left-hand side and the right-hand side for powers of t and comparing we get,

$$\frac{\exp(-\pi\nu_P)}{2\pi i}\oint_\Gamma dz\, z^{i\nu_P}(1-z)^{-i\nu_P}=i\nu_P\; , \tag{80}$$

$$\frac{\exp(-\pi\nu_P)}{2\pi i}\oint_\Gamma dz\, z^{i\nu_P+1}(1-z)^{-i\nu_P}=\tfrac{1}{2}(i\nu_P)(i\nu_P+1)\; . \tag{81}$$

We finally obtain the transition probability from Eq. (78) as

$$\begin{aligned} T_{ij}^{\alpha\beta-}=&\frac{N}{2\pi i}[\exp(-\pi\nu_P)-\exp(\pi\nu_P)]\int_0^1 dz\, z^{i\nu_P}(1-z)^{-i\nu_P}F(z)\\ &+N(i\nu_P)f(0)+\frac{N}{2}(i\nu_P)(i\nu_P+1)[f(1)-f(0)]\; . \end{aligned} \tag{82}$$

To evaluate the one-dimensional integral in Eq. (82) numerically, we change the variable of integration from z to y, using the transformation

$$\exp(y)=(1-z)/z\; , \tag{83}$$

so that the integral $T=\int_0^1 dz\, z^{i\nu_P}(1-z)^{i\nu_P}F(z)$ in (82) reduces to the form

$$T=\int_0^\infty \frac{\exp(-i\nu_P y)}{[1+\exp(y)]}e^yF(y)dy+\int_{-\infty}^0 \frac{\exp(-i\nu_P y)}{[1+\exp(y)]^2}e^yF(y)dy\; . \tag{84}$$

In the second term of (84) we put $y=-y$, and arrive at

$$T=\int_0^\infty \frac{\exp(-i\nu_P y)}{[1+\exp(y)]^2}e^yF(y)dy+\int_0^\infty \frac{\exp(i\nu_P y)}{[1+\exp(-y)]^2}e^{-y}F(-y)dy\; . \tag{85}$$

These two integrals are now evaluated numerically using the Gauss-Laguerre quadrature method. To calculate the total-capture cross sections $Q_{ij}^{\alpha\beta-}$, the Gauss-Legendre quadrature method has been used for the integration over the transverse momentum transfer η. The value of η has been increased stepwise until the desired accuracy of 0.5% in the total-capture cross sections is obtained. In order to check the numerical program developed for the present calculation, some known results[50] for the total-capture cross sections into a few low-lying states have been reproduced.

VI. RESULTS AND DISCUSSIONS

Calculations have been carried out at incident energies between 100 and 1500 keV for capture into all final states with $n \leq 4$ for Li^{3+}-H(1s) collisions. In Table I, we have presented our results for the capture cross sections, $Q(n)=\sum_{lm} Q_{nlm}$, into each complete shell as well as the individual cross sections in each sublevel $Q_{nl}=\sum_m Q_{nlm}$. In order to compare the observed data for the total-capture cross section $Q(\text{total})=\sum_n Q(n)$, a correction term must be made for capture into a higher excited level with $n \geq 5$. In estimating Q(total), we may assume that the cross section $Q(n)$ is proportional to n^{-3} for $n \geq 5$ as in the BK approximation at high energies. This yields

$$Q(\text{total})=\sum_n Q(n) \simeq Q_{1s}+Q_{2s}+Q_{2p}+Q_{3s}+Q_{3p}+Q_{3d}+\frac{Q_{4s}+Q_{4p}+Q_{4d}+Q_{4f}}{Q_{4s}^{\text{BK}}+Q_{4p}^{\text{BK}}+Q_{4d}^{\text{BK}}+Q_{4f}^{\text{BK}}} \sum_{n=4}^{\infty} Q^{\text{BK}}(n)$$

$$=Q(1)+Q(2)+Q(3)+2.561Q(4) . \quad (86)$$

Using the values of $Q(1)$, $Q(2)$, $Q(3)$, and $Q(4)$ obtained by the present CDW approximation, the total-capture cross sections are calculated for each individual energy and are included in Table I. From the table, it appears that throughout the energy region considered the capture into the ground state is almost negligible except at the highest energy of 1500 keV where it amounts to 10% of the total-capture cross section. The small value of ground-state capture is also predicted by Bransden *et al.*,[28] in their calculation for the charge-transfer cross section in the multicharged ion-atom collisions using the atomic-state expansion method and also by Mandal *et al.*,[31] in their calculation of the CB approximation. From the present calculation it appears that in the intermediate-energy region maximum contribution in the capture cross section arises from the $n=3$ level of Li^{2+} ion and this is quite expected since the third-energy level of Li^{2+} ion is in resonance with H(1s) in the capture process, and as the n value increases the capture probability decreases, which is in correspondence with the earlier calculations.[25,28,31] This may be explained as the energy difference between the ground state of atomic hydrogen and $Li^{2+}(nlm)$ ion increases with the increase of n (for $n>3$), the capture cross sections for the levels specified by $n>3$ are expected to be small compared to the resonating level ($n=3$). At higher energies of the projectile, the capture probability is found to be

TABLE I. The present CDW cross section $Q_{nl}(\pi a_0^2)$ for charge transfer in $^7Li^{3+}$ + H(1s)$\rightarrow$$^7Li^{2+}(nl)$+$H^+$ collision.

Energy E in keV	$Q_{1s}\equiv(Q(1))$	Q_{2s}	Q_{2p}	$Q(2)$	Q_{3s}	Q_{3p}	Q_{3d}
100	1.08(−1)[a]	9.26(0)	1.25(1)	2.18(1)	4.48(0)	2.81(1)	7.98(1)
200	1.43(−1)	1.56(0)	7.41(0)	8.97(0)	6.72(−1)	7.07(0)	1.37(1)
400	3.67(−2)	1.76(−1)	2.00(0)	2.17(0)	1.43(−1)	1.30(0)	1.59(0)
800	2.01(−2)	4.62(−2)	2.65(−1)	3.11(−1)	3.21(−2)	1.44(−1)	1.04(−1)
1250	1.33(−2)	1.60(−2)	5.08(−2)	6.68(−2)	8.93(−3)	2.54(−2)	1.29(−2)
1500	9.81(−3)	9.46(−3)	2.39(−2)	3.34(−2)	4.87(−3)	1.16(−2)	5.13(−3)

Energy E in keV	$Q(3)$	Q_{4s}	Q_{4p}	Q_{4d}	Q_{4f}	$Q(4)$	Q(total)
100	1.12(2)	2.79(0)	2.57(1)	3.11(1)	1.82(1)	7.78(1)	3.33(2)
200	2.14(1)	5.03(−1)	5.08(0)	6.87(0)	3.51(0)	1.59(1)	7.15(1)
400	3.03(0)	1.03(−1)	7.99(−1)	9.19(−1)	3.64(−1)	2.18(0)	1.08(1)
800	2.81(−1)	1.89(−2)	7.99(−2)	6.47(−2)	1.77(−2)	1.81(−1)	1.07(0)
1250	4.73(−2)	4.78(−3)	1.32(−2)	8.13(−3)	1.71(−3)	2.78(−2)	1.98(−1)
1500	2.16(−2)	2.52(−3)	5.95(−3)	3.22(−3)	6.16(−4)	1.23(−2)	9.63(−2)

[a]The numbers in parentheses denote the powers of ten by which the numbers are to be multiplied.

maximum at the second quantum level of Li^{2+} ion instead of the resonating level. This is attributed to the fact that at high energy the capture probability is maximum at small values of impact parameter and, consequently, the electron transfer into the inner shells is more dominant. Thus the n-dependent cross sections in the intermediate- and high-energy region can be understood.

At intermediate impact energies, the l-dependent cross sections Q_{nl} indicate a maximum at $l < n-1$ for $n=4$, whereas the results for $n=3$ indicate a maximum at $l=n-1$. In low- and intermediate-energy region the effect of level crossing is responsible for the electron transfer and, consequently, the electron is mostly transferred into a state that has a wave function indicating a large amplitude at the crossing point, which usually has a smaller value of l than $n-1$. At the higher energy, the distributions are completely free from the influence of level crossing, but 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.[25,28,56,57] Although we have not shown the m-dependent cross sections in the present table, it has been found that the distributions over m 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.[25,31]

Belkić *et al.*,[49] gave an estimate for the total-capture cross sections in Li^{3+}-H(1s) collisions, using the relation

$$Q(\text{total}) = Q_{1s}+Q_{2s}+Q_{2p} + 2.081(Q_{3s}+Q_{3p}+Q_{3d}) , \qquad (87)$$

which is obtained by assuming the validity of the n^{-3} scaling law from the level $n>4$. Further, they have not calculated the contribution of capture from the 3d excited state of Li^{2+} ion for total-capture cross sections. In the present investigation we propose to calculate the total-capture cross section Q(total) by using the relation (86) instead of (87). For Li^{3+} projectile, the use of the relation (86) appears to be more justified in Li^{3+}-H(1s) charge exchange because the $n=3$ level is in energy resonance and the effect of resonant behavior of the cross sections for capture into the third quantum level of Li^{2+} ion is manifested in the present calculation even below 800 keV. The values of the total cross sections obtained by the use of (86) is found to be about 9% higher than that obtained by the use of (87) at the incident energy of 1500 keV. At 100 keV, this discrepancy amounts to 24%. The origin for such a difference in the values of the cross sections may be due to the resonant behavior of the electron-capture cross sections for the third quantum level of Li^{2+} ion.

Recently, Shah *et al.*,[6] have empirically found an approximately Z_P^3 scaling law for impact velocity greater than 1 a.u. More recently, Goffe *et al.*,[14] have further confirmed this law experimentally for the impact of fully stripped ions, such as B^{5+}, C^{6+}, N^{7+} ions with atomic hydrogen. However, for the impact of H^+ the cross section becomes too large by as much as a factor of 2 and shows a different velocity dependence. To study the behavior of the cross section as a function of incident charge of the projectile Z_P is of special interest theoretically. We have plotted in Fig. 1 the calculated capture cross sections divided by the cube of the projectile charge $[Q(\text{total})/Z_P^3]$ against the equivalent proton energy obtained by applying the

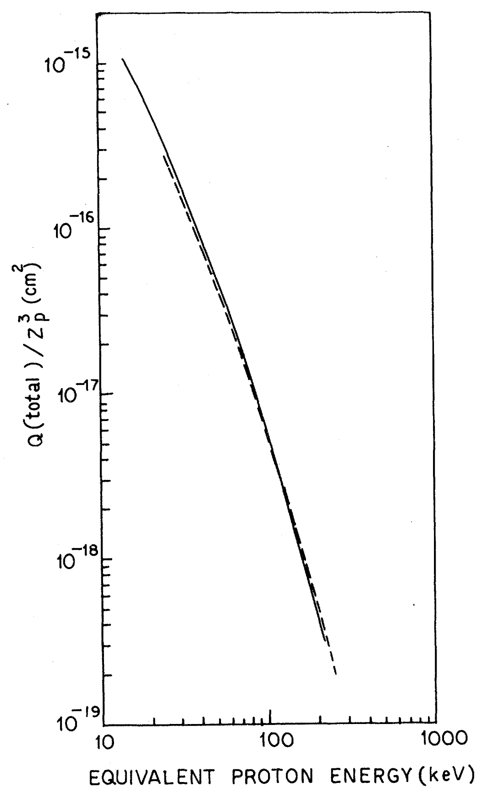

FIG. 1. Ratio of $Q(\text{total})/Z_P^3$ against the equivalent proton energy in the CDW approximation. —, Present results for the projectile Li^{3+}; - - -, CDW calculation for the projectile He^{2+}, Belkić and Gayet, Ref. 48; Belkić and Janev, Ref. 47.

present CDW approximation in Li^{3+}-H(1s) collisions and the previously reported CDW calculations for He^{2+}-H(1s) collisions.[47,48] From Fig. 1, it appears that over an energy range 14–200 keV amu^{-1}, $Q(\text{total})/Z_P^3$ is the same for both the projectiles, He^{2+} and Li^{3+} ions, indicating a Z_P^3 variation of the cross section. For a given relative velocity, Crothers and Todd[58] have also reported that high-energy approximations, such as the BK, CDW, and CIS model lead to a Z_P^3 variation of the cross section. At a very large velocity, the BK cross section[59] is proportional to Z_P^5, however, at lower energies the variation may be closer to Z_P^2 which was predicted by Presnyakov and Ulantsev.[60] The atomic-state expansion method used by Bransden *et al.*,[28] also exhibit roughly Z_P^2 variation of the cross sections over the energy range 10–100 keV amu^{-1}. It is clear that the assumption of proportionality to a power of Z_P is rather too simple and the simultaneous scaling of cross sections and velocities seems to be more accurate as it has been pointed out by Ryufuku and Watanabe[25] and by Gardner *et al.*[10] However, such a procedure is basically an empirical interpolation formula, since there exists no sound theoretical basis to conclude that the velocity should follow the scaling law.

In Fig. 2 we present our theoretical values for the total capture cross section in the energy range 100–1500 keV and have compared them with the recent experimental results of Shah *et al.*,[6] and the previously reported theoretical calculations.[22,25,28,31] The present results obtained by the CDW approximation are found to be in excellent agreement with experimental results in the energy range $E \geq 700$ keV, whereas it grossly overestimates the experimental findings at the lower-energy side ($E < 700$ keV). At 100 keV the calculated results show some discrepancy with the experimental results which is not unlikely because the CDW approximation is a high-energy approximation and is not expected to be valid at low energy. The values of the cross section estimated by the Monte Carlo approach of Olson and Salop[22] show good agreement with the observed values at the lower-energy side up to 300 keV, but beyond that it grossly overestimates the observed findings.[6] Moreover, the shape of the cross section as a function of energy appears rather different; the cross sections decrease with the increase of energy more rapidly showing complete disagreement with the observed trend. This may be attributed to the large statistical errors involved in this calculation.

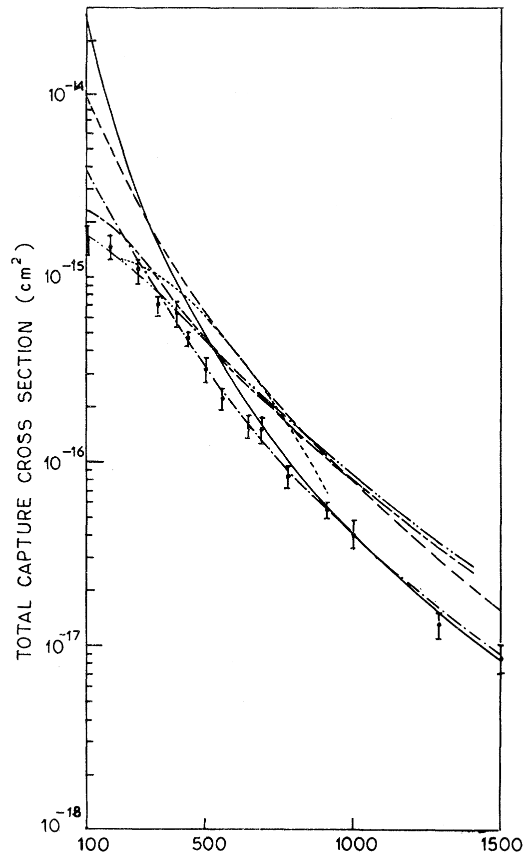

FIG. 2. Total-capture cross section Q(total) for the projectile $^7Li^{3+}$ ion incident on ground-state atomic hydrogen. Theory: —, present CDW approximation; — ·· —, UDWA of Ryufuku and Watanabe, Refs. 25; ---, Monte Carlo method, Olson and Salop, Ref. 22; ——, two-state atomic-expansion method, Bransden *et al.*, Ref. 28; —·—, Coulomb-Born approximation, Mandal *et al.*, Ref. 31; — — —, Born approximation, Mandal *et al.*, Ref. 31. Experiment: · Shah *et al.*, Ref. 6.

The UDWA results of Ryufuku and Watanabe,[25] on the other hand, give quite good agreement in the low-energy region up to the incident energy of 400 keV, but beyond this incident energy the UDWA results grossly overestimate the observed values. This may be due to the fact that all interactions among the product channels are ignored in this method and the results thus obtained are large especially in the high-energy region where the direct excitation channels and the ionization channels significantly influence the cross-section results. The capture cross section in two-state atomic-expansion method used by Bransden *et al.*,[28] agrees rather well in shape with the experimental data but always overestimates the data in the intermediate- and high-energy region. The UDWA cross sections, although agree well with the two-state cross sections of Bransden *et al.*,[28] at the higher energies, are considerably smaller at the lower energies. The cross sections obtained by the CB approximation[31] are found to be in very good agreement with the experimental results[6] throughout the energy region considered except at the very-low-energy region $E < 275$ keV, whereas the Born cross sections grossly overestimate the total cross sections throughout the energy region considered.

However, a rigorous close-coupling approximation based on the atomic-state expansion method at the intermediate-energy region could give more reliable results for the cross sections. The increasing number of open channels in this energy region makes the coupled-channel calculations almost untenable for highly charged ion-atom collisions. Thus, in view of the success in predicting the cross sections for Li^{3+}-H collisions in the intermediate- and high-energy region, the CDW approximation is highly encouraging to give an estimate for the capture cross sections for highly stripped ion-atom collisions as compared to the close-coupling calculations.

VII. CONCLUSIONS

The present method of calculation provides an alternative way for the evaluation of the CDW scattering amplitude. It does not require the imposition of any restriction on the values of the quantum numbers n, l, and m of the excited state and also on the charge of the incident projectile. In this proposed method the exchange scattering amplitude has been reduced to a one-dimensional integral in real space which can be very easily evaluated numerically. As a result, we obtain more detailed theoretical predictions, which, in turn, might be checked with the experimental observations on radiative transitions and radiative cascades following electron capture. The influence of inelastic intermediate channels describing excitation and ionization on the charge-transfer processes is expected to be considerable at high-impact energies. At high-incident velocities, all intermediate channels are open and it is likely that the charge-exchange process should be significantly affected by the inclusion of these intermediate states. The main feature of the CDW approach is that it takes into account the continuum intermediate states in the charge-exchange process ensuring the correct initial- and final-state boundary conditions of the problem. The present method for obtaining the cross sections for capture into n, l, and m states of the projectiles may be helpful for the diagonostic techniques for studying the role played by the impurities in neutral-beam heating of fusion plasmas.

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