

# Electron capture in collisions of $\text{He}^{2+}$ with Li atoms and of $\text{Li}^{3+}$ , $\text{C}^{6+}$ , and $\text{O}^{8+}$ with He atoms in the high-energy region

G. C. Saha

*Department of Physics, Fakirchand College, Diamond Harbour 743 331, West Bengal, India*

Shyamal Datta and S. C. Mukherjee

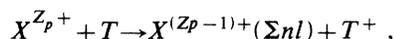
*Department of Theoretical Physics, Indian Association for the Cultivation of Science, Jadaupur, Calcutta 700 032, India*

(Received 15 January 1986)

A method has been developed for the evaluation of the Coulomb integrals containing the product of the Coulomb wave function with Slater-type orbitals which serve as the basis set in constructing the wave function of multielectron atoms within the self-consistent-field approximation, in terms of the Gauss hypergeometric function for an arbitrary  $nlm$  state. Analytical expressions are derived for the integrals in closed form irrespective of either the triad  $nlm$  or of the quantization axis. This method has been applied in the framework of continuum distorted-wave approximation to obtain the charge-transfer cross section in various collision cases involving heavy stripped ions and multielectron targets. The calculated results are found to be in good agreement with the recent experimental findings and the existing theoretical calculations in the high-energy region.

## I. INTRODUCTION

The theoretical and experimental study of charge-transfer processes from multielectron atoms has recently added a new dimension to the problem and hence attracted a great deal of attention because of the importance of charge-transfer cross sections in connection with the diagnostics of fusion plasma.<sup>1</sup> The reactions to be studied are of the form



where  $X^{Z_p+}$  represents the incident ion and  $T$  represents the multielectron target. As the incident ion is fully stripped,  $Z_p$  is equal to the nuclear charge, the ion  $X^{(Z_p-1)+}$  becomes hydrogenic and is characterized by a set of single-electron quantum numbers  $nlm$ .

In this paper we present the cross sections calculated for single-electron capture from the tightly bound  $K$  shell of the He and Li atom and also from the loosely bound valence electron ( $L$  shell) of the Li atom in collisions of  $\text{Li}^{3+}$ ,  $\text{C}^{6+}$ ,  $\text{O}^{8+}$  with He atom as well as of the  $\text{He}^{2+}$  with the Li atom in the framework of the continuum distorted-wave approximation (CDWA). From the viewpoint of the scattering theory, the most adequate methods are certainly the impulse approximation<sup>2-4</sup> (IA), the continuum distorted-wave (CDW) method,<sup>5,6</sup> and the strong potential Born approximation (SPBA). Since the CDW method preserves the correct boundary conditions for the charge-exchange problem, the distortion of the wave functions due to the internuclear Coulomb potential and the interactions between the electron to be captured and the nuclei are properly taken into account, it follows from the quantal version of Gayet,<sup>7</sup> that CDW approximation is the rigorous first-order term of a perturbation series.

We propose to develop a method for the calculations of

cross sections for electron capture from the inner shells of a complex atom into arbitrary  $n$ ,  $l$ , and  $m$  states of fast projectiles in collision of fully stripped ion with a multielectron target in the framework of the CDW approximation. The effects of continuum intermediate states are properly taken into account<sup>8</sup> in describing a charge-transfer reaction at high energy. We consider the active electron moving in the field of an effective nuclear charge and expand the bound-state wave function of complex atoms on to the basis of Slater-type orbitals.<sup>9</sup>

Recently, with the advent of multiply charged ion sources, theoretical interest has been focused on the investigations of various multicharged ion-atom collision processes. However, quantal calculations suffer from serious computational difficulties; as the projectile charge increases, the electrons are captured into increasingly higher principal shells of the projectile. As a result, theoretical studies in the quantum mechanical approach are only a few. On the other hand, some classical and semiclassical approaches have recently been suggested so as to determine the capture cross sections for the heavy-stripped-ion-atom collisions. Olson<sup>10</sup> applied a classical trajectory Monto Carlo method (CTMC) to calculate the charge-transfer cross section between the  $\text{He}^{2+}$  ion and Li atom. Suzuki *et al.*<sup>11</sup> also applied the unitarized distorted-wave approximation (UDWA) to study the capture cross sections between  $\text{Li}^{3+}$ ,  $\text{C}^{6+}$ ,  $\text{O}^{8+}$  ions with the He atom. Ermolaev and Bransden<sup>12</sup> have also extended their two-state impact-parameter method to measure the capture cross section in the  $\text{He}^{2+} + \text{Li}$  collisions. It is observed from their calculations that in the energy region of 1000 keV the charge exchange is dominated by capture of electrons from the  $K$  shell of Li atoms. Recently, Sidorovich *et al.*<sup>13</sup> have applied the approximation of Bassel and Gerjuoy<sup>14</sup> to calculate the charge-changing cross sections in collisions of  $\text{H}^+$ ,  $\text{He}^{2+}$ , and  $\text{Li}^{3+}$  ions with He atoms in the energy region of 0.025–4 MeV/amu in the

independent-electron approximation.

Because of the formidable difficulties due to many-electron effects, a single-electron model has been adopted to carry out the theoretical study of electron-capture cross section in ion-atom collisions. The existing theoretical calculations<sup>7,8,10,15-21</sup> also are based on the independent-particle model which is justified due to the wide separation of binding energies for the inner subshell electrons. The wave functions of the target atoms have been represented by unmodified hydrogenic wave functions and the experimental binding energies in conjunction with the effective charges have been used in those calculations. As the charge of the incident particle increases, capture cross sections will dominate from higher values of the principal quantum number  $n$  of the captured states. The calculation of cross sections for such high quantum states normally involves the process of repeated parametric differentiation of the relevant generating function. Belkić, Gayet, and Salin<sup>8</sup> have used this technique to calculate the charge transfer cross section in the ion-atom collisions. Recently, a closed-form expression of the Coulomb integrals which are of direct use for charge transfer in the CDW method has been derived by Belkić<sup>22</sup> in spherical coordinates in terms of Appell hypergeometric polynomials of two variables. These generalized Coulomb integrals have also been calculated by Belkić<sup>23</sup> in a closed form in terms of a linear combination of hypergeometric polynomials of two and three variables and by Dubé<sup>24</sup> in terms of the Gauss hypergeometric function for arbitrary  $nlm$  by the use of parabolic coordinates. On the other hand, we express the Coulomb integrals in terms of a terminating hypergeometric series which is more convenient for the calculation of cross sections for capture into arbitrary  $n$ ,  $l$ , and  $m$  states of the fast, fully stripped projectiles from the multielectron atoms. We have compared our theoretical results with the recent experimental findings of Shah and co-workers,<sup>25,26</sup> Nikolaev *et al.*,<sup>27</sup> Pivovar, Levchenko, and Krivonosov,<sup>28</sup> Macdonald and Martin,<sup>29</sup> Hippler *et al.*,<sup>30</sup> Dillingham, Macdonald, and Richard,<sup>31</sup> and McCullough *et al.*<sup>32</sup>

In Sec. II we outline the general expression for the CDWA scattering amplitude into arbitrary  $n, l, m$  states 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 experimental findings and available theoretical calculations. Finally, in Sec. IV a concluding summary of the present investigations is described. Atomic units are used throughout the paper, unless otherwise stated.

## II. THEORY

### A. General expression of the CDW electron-capture cross sections

The prior form<sup>8</sup> of the CDW cross sections  $Q_{if}^-$  for electron capture by fast bare projectiles from the multielectron atoms within the framework of independent-electron model can be written as

$$Q_{if}^-(a_0^2) = \frac{1}{\pi} (2\pi v)^{-2} \int d\boldsymbol{\eta} |T_{if}^-(\boldsymbol{\eta})|^2,$$

where  $\boldsymbol{\eta}$  is the usual transverse momentum transfer perpendicular to the incident velocity  $\mathbf{v}$  of the projectile and  $T_{if}^-$  is the transition amplitude

$$T_{if}^- = -N(v)\mathbf{J} \cdot \mathbf{K}, \quad (1)$$

with

$$\mathbf{J} = \int d\mathbf{x} \exp(i\mathbf{p} \cdot \mathbf{x}) [\nabla_{\mathbf{x}} \Phi_i(\mathbf{x})] {}_1F_1(i\nu_i; 1; i\nu\mathbf{x} + i\mathbf{v} \cdot \mathbf{x}), \quad (2)$$

$$\mathbf{K} = \int d\mathbf{s} \exp(i\mathbf{q} \cdot \mathbf{s}) \Phi_f^*(\mathbf{s}) \nabla_{\mathbf{s}} {}_1F_1(i\nu_p; 1; i\nu\mathbf{s} + i\mathbf{v} \cdot \mathbf{s}), \quad (3)$$

$$N(v) = \Gamma(1 - i\nu_i) \Gamma(1 - i\nu_p) \exp\left[\frac{1}{2}\pi(\nu_p + \nu_i)\right], \quad (4)$$

$$\mathbf{p} = -\boldsymbol{\eta} - \left[ \frac{\varepsilon_i - \varepsilon_f}{v^2} + 1/2 \right] \mathbf{v}, \quad (5)$$

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

$$\nu_p = Z_p/v, \quad (7)$$

$$\nu_i = Z_i^*/v. \quad (8)$$

Here  $\varepsilon_i$  is the Roothan-Hartree-Fock (RHF) energy corresponding to the RHF orbital  $\Phi_i(\mathbf{x})$  of the active electron.  $\varepsilon_f$  and  $\Phi_f(\mathbf{s})$  correspond, respectively, to the energy and wave function in the final state of the hydrogenic ion.  $Z_p$  represents the charge of the projectile and  $Z_i^*$  is the effective nuclear charge of the target atom related with the principal quantum number  $n_i$  of the active electron by the relation

$$Z_i^* = (-2n_i\varepsilon_i)^{1/2}. \quad (9)$$

The wave function of the multielectron atom may be expanded onto the basis of Slater-type orbitals as

$$\Phi_i(\mathbf{x}) = \sum C_i \chi_i(\mathbf{x}), \quad (10)$$

where the basis functions  $\chi_i(\mathbf{x})$  represents the normalized Slater-type orbitals in spherical coordinates

$$\chi_i(\mathbf{x}) = N_{\alpha_i} x^{n_i-1} e^{-\alpha_i x} Y_{l_i m_i}(\hat{\mathbf{x}}), \quad (11)$$

with

$$N_{\alpha_i} = [(2\alpha_i)^{2n_i+1} / (2n_i)!]^{1/2}, \quad (12)$$

$\alpha_i$  being a variational parameter associated with the orbital quantum number  $n_i$ .

### B. Evaluation of the integral $\mathbf{J}$

We make use of the Fourier theorem<sup>33</sup>

$$\int d\mathbf{r} e^{i\mathbf{q} \cdot \mathbf{r}} \nabla_{\mathbf{r}} f(\mathbf{r}) = \left[ \frac{1}{i} \right] \mathbf{q} \int d\mathbf{r} e^{i\mathbf{q} \cdot \mathbf{r}} f(\mathbf{r}),$$

where  $f(\mathbf{r})$  is any integrable function, and obtain the  $\mathbf{J}$  integral in Eq. (2) as

$$\mathbf{J} = \mathbf{J}_1 - \mathbf{J}_2, \quad (13)$$

where

$$\mathbf{J}_1 = i\mathbf{p} \int d\mathbf{x} e^{-i\mathbf{p}' \cdot \mathbf{x}} \Phi_i(\mathbf{x}) {}_1F_1(i\nu_i; 1; i\nu\mathbf{x} + i\mathbf{v} \cdot \mathbf{x}), \quad (14)$$

$$\mathbf{J}_2 = \int d\mathbf{x} e^{-i\mathbf{p}'\cdot\mathbf{x}} \Phi_i(\mathbf{x}) \nabla_{\mathbf{x}} {}_1F_1(iv_t; 1; i\mathbf{v}\cdot\mathbf{x}), \quad (15)$$

with

$$\mathbf{p}' = -\mathbf{p}. \quad (16)$$

The reduction of the integral  $\mathbf{J}_1$  in Eq. (14) can be performed easily in a terminating hypergeometric series following a procedure similar to Saha *et al.*<sup>20</sup> assuming our axis of quantization along the direction of  $\mathbf{v}$ . We obtain

$$\begin{aligned} \mathbf{J}_1 = & i\mathbf{p}' 4\pi(2i)^{l_i} \sum_i \sum_{\delta_i=0}^{[(n_i-l_i)/2]} \sum_{w_i=0}^{n_i-l_i-2\delta_i} \sum_{l'_i=0}^{l_i} C_i N_{\alpha_i} (-1)^{-\delta_i} \frac{(n_i-l_i)!(n_i-\delta_i)!}{(2\delta_i)!(n_i-l_i-2\delta_i-w_i)!w_i!} \\ & \times 2^{n_i-l_i-\delta_i} N_{l'_i l'_i} d^{w_i} c^{n_i-l_i-2\delta_i-w_i} a^{-(n_i-\delta_i+1)} \frac{(i\nu_t)^{w_i+l'_i}}{(w_i+l'_i)!} \left[1 - \frac{b}{a}\right]^{-n_i+\delta_i-i\nu_t} \\ & \times {}_2F_1 \left[ w_i+l'_i-n_i+\delta_i, 1-i\nu_t, w_i+l'_i+1, \frac{b}{a} \right], \end{aligned} \quad (17)$$

where

$$a = \alpha_i^2 + p'^2, \quad (18)$$

$$b = 2i\alpha_i v + 2\mathbf{p}'\cdot\mathbf{v}, \quad (19)$$

$$c = \alpha_i, \quad (20)$$

$$d = -iv, \quad (21)$$

$$N_{l'_i l'_i} = (-1)^{l''_i} v^{l'_i} (p')^{l''_i} Y_{l'_i 0}(\hat{\mathbf{v}}) Y_{l'_i m_i}(\hat{\mathbf{p}}') \left[ \frac{4\pi(2l_i+1)(l_i-|m_i|)!(l_i+|m_i|)!}{(2l'_i+1)(2l''_i+1)(l''_i-|m_i|)!(l'_i!)^2(l''_i+|m_i|)!} \right]^{1/2}, \quad (22)$$

$$l''_i = l_i - l'_i, \quad (23)$$

and  $[(n_i-l_i)/2]$  being the largest integer less than or equal to  $(n_i-l_i)/2$ . The  $\mathbf{J}_2$  integral in Eq. (15) may be expressed as

$$\mathbf{J}_2 = v \nabla_{\mathbf{v}} \int d\mathbf{x} \frac{e^{-i\mathbf{p}'\cdot\mathbf{x}}}{x} \Phi_i(\mathbf{x}) {}_1F_1(iv_t; 1; i\mathbf{v}\cdot\mathbf{x}), \quad (24)$$

with  $p'$  and  $\nu_t$  taken as parameters independent of  $v$ . We use the integral representation<sup>20</sup> for the confluent hypergeometric function and the space part of the integration in Eq. (24) yields

$$\mathbf{J}_2 = 4\pi v \nabla_{\mathbf{v}} \sum_i C_i N_{\alpha_i} (2i)^{l_i} l_i! \frac{1}{2\pi i} \oint_{\Gamma} dt p(t, \nu_t) Q^{l_i} Y_{l_i m_i}(\hat{\mathbf{Q}}) \left[ -\frac{\partial}{\partial \mu} \right]^{n_i-l_i-1} (\mu^2 + Q^2)^{-(l_i+1)}, \quad (25)$$

where

$$p(t, \nu_t) = t^{i\nu_t-1} (t-1)^{-i\nu_t}, \quad (26)$$

$$\mu = \alpha_i - ivt, \quad (27)$$

$$\mathbf{Q} = \mathbf{v}t - \mathbf{p}'. \quad (28)$$

We apply the procedure of Todd *et al.*<sup>34</sup> for the  $(n_i-l_i-1)$ th-order differentiation with respect to  $\mu$  in Eq. (25) and obtain the  $\mathbf{J}_2$  integral as

$$\begin{aligned} \mathbf{J}_2 = & 4\pi v \nabla_{\mathbf{v}} \sum_i C_i N_{\alpha_i} (2i)^{l_i} \frac{1}{2\pi i} \sum_{\delta_i=0}^{[(n_i-l_i-1)/2]} (-1)^{2n_i-2l_i-2-\delta_i} \frac{(n_i-l_i-1)!(n_i-\delta_i-1)!}{(n_i-l_i-1-2\delta_i)!(2\delta_i)!} 2^{n_i-l_i-\delta_i-1} \\ & \times \oint_{\Gamma} dt p(t, \nu_t) Q^{l_i} Y_{l_i m_i}(\hat{\mathbf{Q}}) \mu^{n_i-l_i-2\delta_i-1} (\mu^2 + Q^2)^{-(n_i-\delta_i)}, \end{aligned} \quad (29)$$

where  $[(n_i-l_i-1)/2]$  represents the largest integer less than or equal to  $(n_i-l_i-1)/2$ . We now take the binomial expansion of  $(\mu^2 + Q^2)^{-(n_i-\delta_i)}$  and  $\mu^{n_i-l_i-2\delta_i-1}$  and use the addition theorem for regular solid harmonics<sup>35</sup> and obtain the  $\mathbf{J}_2$  integral in an arbitrary quantization axis as

$$\begin{aligned}
\mathbf{J}_2 = & 4\pi v \nabla_v \sum_{\delta_i=0}^{[(n_i-l_i-1)/2]} \sum_{l'_i=0}^{l_i} \sum_{m'_i=-l'_i}^{l'_i} \sum_{w_i=0}^{(n_i-l_i-2\delta_i-1)} C_i N_{\alpha_i} 4\pi(2i)^{l_i} (-1)^{-\delta_i} 2^{n_i-l_i-1-\delta_i} v^{l'_i} Y_{l'_i m'_i}(\hat{\mathbf{v}}) M_{l'_i l'_i} \\
& \times \frac{(n_i-l_i-1)(n_i-\delta_i-1)!}{(2\delta_i!!)(n_i-l_i-1-2\delta_i-w_i)! w_i!} d^{w_i} c^{n_i-l_i-1-2\delta_i-w_i} \\
& \times a^{-(n_i-\delta_i)} \sum_{u=0}^{\infty} \frac{(n_i-\delta_i)_u}{u!} \left[ \frac{b}{a} \right]^u \frac{1}{2\pi i} \\
& \times \oint_{\Gamma} dt (t-1)^{-i\nu_t} t^{-1+i\nu_t+l'_i+w_i+u}, \quad (30)
\end{aligned}$$

where

$$M_{l'_i l'_i} = (-1)^{l'_i} \left[ \frac{l_i + |m'_i|}{l'_i + |m'_i|} \right] (p')^{l'_i} Y_{l'_i m'_i}(\hat{\mathbf{p}}') \left[ \frac{4\pi(l'_i + |m'_i|)(l'_i + |m''_i|)(2l_i+1)(l_i - |m_i|)!}{(2l''_i+1)(l'_i - |m''_i|)(l_i + |m_i|)(2l_i+1)(l'_i - |m'_i|)!} \right]^{1/2}, \quad (31)$$

$$l''_i = l_i - l'_i, \quad (32)$$

$$m''_i = m_i - m'_i, \quad (33)$$

and  $a$ ,  $b$ ,  $c$ , and  $d$  are defined in Eqs. (18)–(21). The contour integration in Eq. (30) can be performed easily, which can be expressed in a closed form as

$$\begin{aligned}
\mathbf{J}_2 = & \sum_i \sum_{\delta_i=0}^{[(n_i-l_i-1)/2]} \sum_{l'_i=0}^{l_i} \sum_{m'_i=-l'_i}^{l'_i} \sum_{w_i=0}^{n_i-l_i-2\delta_i-1} C_i N_{\alpha_i} 4\pi v (2i)^{l_i} (-1)^{-\delta_i} 2^{n_i-l_i-1-\delta_i} \frac{(n_i-l_i-1)(n_i-\delta_i-1)!}{(2\delta_i!!)(n_i-l_i-1-2\delta_i-w_i)! w_i! (w_i+l'_i)!} \\
& \times M_{l'_i l'_i} c^{n_i-l_i-1-2\delta_i-w_i} a^{-(n_i-\delta_i)} (i\nu_t)_{w_i+l'_i} \\
& \times \left\{ \nabla_v \left[ d^{w_i} {}_2F_1 \left[ n_i-\delta_i, i\nu_t+l'_i+w_i, w_i+l'_i+1, \frac{b}{a} \right] v^{l'_i} Y_{l'_i m'_i}(\hat{\mathbf{v}}) \right] \right\}. \quad (34)
\end{aligned}$$

Now we apply the  $\nabla_v$  operator in Eq. (34) and then choose our axis of quantization along the direction of  $\mathbf{v}$  and obtain the  $\mathbf{J}_2$  integral in a terminating hypergeometric series as

$$\begin{aligned}
\mathbf{J}_2 = & \sum_i \sum_{\delta_i=0}^{[(n_i-l_i-1)/2]} \sum_{l'_i=0}^{l_i} \sum_{w_i=0}^{n_i-l_i-2\delta_i-1} C_i N_{\alpha_i} 4\pi v (2i)^{l_i} (-1)^{-\delta_i} 2^{n_i-l_i-1-\delta_i} \frac{(n_i-l_i-1)(n_i-\delta_i-1)!}{(2\delta_i!!)(n_i-l_i-1-2\delta_i-w_i)! w_i! (w_i+l'_i)!} M_{l'_i l'_i} \\
& \times c^{n_i-l_i-1-2\delta_i-w_i} a^{-(n_i-\delta_i)} (i\nu_t)_{w_i+l'_i} \\
& \times [M_1(p'_x + ip'_y)^{m_i}(i\alpha_i \hat{\mathbf{v}} + \mathbf{p}') + M_2(p'_x + ip'_y)^{m_i-1}(\hat{\mathbf{i}} + i\hat{\mathbf{j}}) \\
& + (p'_x + ip'_y)^{m_i}(M_3 \hat{\mathbf{k}} + M_4 \mathbf{v} + M_5 \mathbf{v})], \quad (35)
\end{aligned}$$

where

$$N_1(m'_i) = (-1)^{l'_i} \left[ \frac{l_i + |m_i|}{l'_i + |m'_i|} \right] \left[ \frac{4\pi(l'_i + |m'_i|)(l'_i + |m''_i|)(2l_i+1)(l_i - |m_i|)!}{(2l''_i+1)(l'_i - |m''_i|)(l_i + |m_i|)(2l_i+1)} \frac{1}{(l'_i - |m'_i|)!} \right]^{1/2}, \quad (36)$$

$$N_2(m'_i) = N_{yl'_i m'_i} \sum_{K=0}^{[(l'_i-m'_i)/2]} (-1)^K \frac{(2l'_i-2K)!}{2^{l'_i} (l'_i-K)(l'_i-m'_i-2K)! K!} (p'_z)^{l'_i-m'_i-2K} p'^{2K}, \quad (37)$$

$$M_1 = N_1(m'_i=0)N_2(m'_i=0)d^{w_i}v^{l'_i}Y_{l'_i 0}(\hat{\nu})2a^{-1}\left[1-\frac{b}{a}\right]^{\delta_i-n_i-iv_i} \\ \times \frac{(n_i-\delta_i)(iv_i+l'_i+w_i)}{(w_i+l'_i+1)} {}_2F_1\left[w_i+l'_i+1-n_i+\delta_i, 1-iv_i, w_i+l'_i+2, \frac{b}{a}\right], \quad (38)$$

$$C_1(m'_i) = N_{y l'_i m'_i} \sum_{K=0}^{[(l'_i-m'_i)/2]} (-1)^K \frac{(2l'_i-2K)!}{2^{l'_i}(l'_i-K)!(l'_i-m'_i-2K)!K!}, \quad (39)$$

$$N_{y l'_i m'_i} = \varepsilon \left[ \frac{(2l'_i+1)(l'_i-|m'_i|)!}{4\pi(l'_i+|m'_i|)!} \right]^{1/2}, \quad (40)$$

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

$$M_2 = N_1(m'_i=1)N_2(m'_i=1)d^{w_i}C_1(m'_i=1)v^{l'_i-1}\left[1-\frac{b}{a}\right]^{\delta_i-n_i+1-iv_i} {}_2F_1\left[w_i+l'_i+1-n_i+\delta_i, 1-iv_i, w_i+l'_i+1, \frac{b}{a}\right], \quad (41)$$

$$C_2(m'_i) = N_{y l'_i m'_i} \sum_{K=0}^{[(l'_i-m'_i)/2]} (-1)^K \frac{(2l'_i-2K)!2K}{2^{l'_i}(l'_i-K)!(l'_i-m'_i-2K)!K!}, \quad (42)$$

$$C_3(m'_i) = N_{y l'_i m'_i} \sum_{K=0}^{[(l'_i-m'_i)/2]} (-1)^K \frac{(2l'_i-2K)!(l'_i-2K)}{2^{l'_i}(l'_i-K)!(l'_i-m'_i-2K)!K!}, \quad (43)$$

$$M_3 = N_1(m'_i=0)N_2(m'_i=0)C_3(m'_i=0)v^{l'_i-1}d^{w_i}\left[1-\frac{b}{a}\right]^{\delta_i-n_i+1-iv_i} {}_2F_1\left[w_i+l'_i+1-n_i+\delta_i, 1-iv_i, w_i+l'_i+1, \frac{b}{a}\right], \quad (44)$$

$$M_4 = N_1(m'_i=0)N_2(m'_i=0)C_2(m'_i=0)v^{l'_i-2}d^{w_i}\left[1-\frac{b}{a}\right]^{\delta_i-n_i+1-iv_i} {}_2F_1\left[w_i+l'_i+1-n_i+\delta_i, 1-iv_i, w_i+l'_i+1, \frac{b}{a}\right], \quad (45)$$

$$M_5 = N_1(m'_i=0)N_2(m'_i=0)v^{l'_i+w_i-2}Y_{l'_i 0}(\hat{\nu})(-i)^{w_i}w_i\left[1-\frac{b}{a}\right]^{\delta_i-n_i+1-iv_i} \\ \times {}_2F_1\left[w_i+l'_i+1-n_i+\delta_i, 1-iv_i, w_i+l'_i+1, \frac{b}{a}\right], \quad (46)$$

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

### C. Evaluation of the integral $\mathbf{K}$

The  $\mathbf{K}$  integral in Eq. (3) may be expressed as

$$\mathbf{K} = v \nabla_v \int d\mathbf{s} \frac{e^{i\mathbf{q}\cdot\mathbf{s}}}{s} \Phi_f^*(\mathbf{s}) {}_1F_1(iv_p; 1; i\mathbf{v}\cdot\mathbf{s}), \quad (47)$$

with  $q$  and  $v_p$  taken as parameters independent of  $v$ . The final bound-state wave function characterized by the set of quantum numbers  $n_f$ ,  $l_f$ , and  $m_f$  may be written as

$$\Phi_f(\mathbf{s}) = R_{n_f l_f}(s) Y_{l_f m_f}(\hat{\mathbf{s}}), \quad (48)$$

where the radial part is given explicitly by

$$R_{n_f l_f}(\mathbf{s}) = - \left[ \left[ \frac{2Z_p}{n_f} \right]^3 \frac{(n_f-l_f-1)!}{2n_f[(n_f+l_f)!]^3} \right]^{1/2} e^{-(1/2)\rho} \rho^{l_f} L_{n_f+l_f}^{2l_f+1}(\rho), \quad (49)$$

$$L_{n_f+l_f}^{2l_f+1}(\rho) = \sum_{k_f=0}^{n_f-l_f-1} (-1)^{k_f+2l_f+1} \frac{[(n_f+l_f)!]^2 \rho^{k_f}}{(n_f-l_f-1-k_f)!(2l_f+1+k_f)!k_f!}, \quad (50)$$

$$\rho = \gamma s, \quad (51)$$

$$\gamma = 2Z_p/n_f. \quad (52)$$

We follow the same procedure<sup>20</sup> for the evaluation of the  $J_2$  integral in Eq. (24) and obtain the  $K$  integral in Eq. (47) as

$$\begin{aligned}
 \mathbf{K} = & - \left[ \frac{\gamma^3(n_f - l_f - 1)!(n_f + l_f)!}{2n_f} \right]^{1/2} 4\pi v(2i)^{l_f} \\
 & \times \sum_{k_f=0}^{n_f - l_f - 1} \sum_{\delta_f=0}^{[k_f/2]} \sum_{w_f=0}^{k_f - 2\delta_f} \sum_{l'_f=0}^{l_f} (-1)^{k_f + 1 + l'_f - \delta_f} \gamma^{l_f + k_f} \\
 & \times \left[ \frac{4\pi(2l_f + 1)(l_f - |m_f|)!(l_f + |m_f|)!}{(2l'_f + 1)(2l'_f + 1)} \right]^{1/2} \\
 & \times \frac{2^{k_f - \delta_f} k_f!(l_f + k_f - \delta_f)!(i\nu_p)_{l'_f + w_f}}{(n_f - l_f - 1 - k_f)!(2l_f + 1 + k_f)!k_f!} \frac{c_1^{k_f - 2\delta_f - w_f} a_1^{-(l_f + k_f - \delta_f + 1)}}{(l'_f + w_f)!(2\delta_f!)w_f!(k_f - 2\delta_f - w_f)!} \\
 & \times \{ M_{1f}(q'_x - iq'_y)^{m_f}(i\lambda\hat{\mathbf{v}} + \mathbf{q}') + M_{2f}(q'_x - iq'_y)^{m_f - 1}(\hat{\mathbf{i}} - i\hat{\mathbf{j}}) \\
 & + (q'_x - iq'_y)^{m_f} [M_{3f}\hat{\mathbf{k}} + \mathbf{v}(M_{4f} + M_{5f})] \} , \tag{53}
 \end{aligned}$$

where

$$a_1 = \lambda^2 + q^2, \tag{54}$$

$$b_1 = 2i\lambda v - 2\mathbf{q} \cdot \mathbf{v}, \tag{55}$$

$$c_1 = \lambda, \tag{56}$$

$$d_1 = -iv, \tag{57}$$

$$\lambda = \gamma/2, \tag{58}$$

$$\mathbf{q}' = -\mathbf{q}, \tag{59}$$

$$A = N_{yl'_f m'_f} \sum_{K=0}^{[(l'_f - m'_f)/2]} (-1)^K (q'_z)^{l'_f - m'_f - 2K} (q')^{2K} \frac{(2l'_f - 2K)!}{2^{l'_f} (l'_f - K)!(l'_f - m'_f - 2K)!K!}, \tag{60}$$

$$B = 1.0 / [(l'_f + |m'_f|)!(l'_f + |m'_f|)!(l'_f - |m'_f|)!(l'_f - |m'_f|)!]^{1/2}, \tag{61}$$

$$C = N_{yl'_f m'_f} \sum_{K=0}^{[(l'_f - m'_f)/2]} (-1)^K \frac{(2l'_f - 2K)!}{2^{l'_f} (l'_f - K)!(l'_f - m'_f - 2K)!K!}, \tag{62}$$

$$N_{yl'_f m'_f} = \varepsilon_1 \left[ \frac{(2l'_f + 1)(l'_f - |m'_f|)!}{4\pi(l'_f + |m'_f|)!} \right]^{1/2}, \tag{63}$$

with  $\varepsilon_1 = (-1)^{m'_f}$  for  $m'_f > 0$  and  $\varepsilon_1 = 1$  for  $m'_f \leq 0$ ,

$$N_{yl'_f m'_f} = \varepsilon_2 \left[ \frac{(2l'_f + 1)(l'_f - |m'_f|)!}{4\pi(l'_f + |m'_f|)!} \right]^{1/2}, \tag{64}$$

with  $\varepsilon_2 = (-1)^{m'_f}$  for  $m'_f > 0$  and  $\varepsilon_2 = 1$  for  $m'_f \leq 0$ ,

$$l'_f = l_f - l'_f, \tag{65}$$

$$m'_f = m_f - m'_f, \tag{66}$$

$$\begin{aligned}
 M_{1f} = & A(m'_f = 0)B(m'_f = 0)d_1^{w_f} v^{l'_f} Y_{l'_f 0}(\hat{\mathbf{v}}) 2a_1^{-1} \left[ 1 - \frac{b_1}{a_1} \right]^{\delta_f - l_f - k_f - i\nu_p - 1} \\
 & \times \frac{(l_f + k_f - \delta_f + 1)(i\nu_p + l'_f + w_f)}{(l'_f + w_f + 1)} {}_2F_1 \left[ l'_f + w_f - l_f - k_f + \delta_f, 1 - i\nu_p, l'_f + w_f + 2, \frac{b_1}{a_1} \right], \tag{67}
 \end{aligned}$$

$$M_{2f} = A(m'_f=1)B(m'_f=1)C(m'_f=1)v^{l'_f-1}d_1^{w_f} \left[ 1 - \frac{b_1}{a_1} \right]^{\delta_f - l_f - k_f - i\nu_p} \\ \times {}_2F_1 \left[ l'_f + w_f - l_f - k_f + \delta_f, 1 - i\nu_p, l'_f + w_f + 1, \frac{b_1}{a_1} \right], \quad (68)$$

$$D = N_{yl'_fm'_f} \sum_{K=0}^{[(l'_f - m'_f)/2]} (-1)^K \frac{(2l'_f - 2K)!(l'_f - 2K)}{2^{l'_f}(l'_f - K)!(l'_f - m'_f - 2K)!K!}, \quad (69)$$

$$M_{3f} = A(m'_f=0)B(m'_f=0)D(m'_f=0)v^{l'_f-1}d_1^{w_f} \left[ 1 - \frac{b_1}{a_1} \right]^{\delta_f - l_f - k_f - i\nu_p} \\ \times {}_2F_1 \left[ l'_f + w_f - l_f - k_f + \delta_f, 1 - i\nu_p, l'_f + w_f + 1, \frac{b_1}{a_1} \right], \quad (70)$$

$$M_{4f} = A(m'_f=0)B(m'_f=0)E(m'_f=0)v^{l'_f-2}d_1^{w_f} \left[ 1 - \frac{b_1}{a_1} \right]^{\delta_f - l_f - k_f - i\nu_p} \\ \times {}_2F_1 \left[ l'_f + w_f - l_f - k_f + \delta_f, 1 - i\nu_p, l'_f + w_f + 1, \frac{b_1}{a_1} \right], \quad (71)$$

$$E = N_{yl'_fm'_f} \sum_{K=0}^{[(l'_f - m'_f)/2]} (-1)^K \frac{(2l'_f - 2K)!2K}{2^{l'_f}(l'_f - K)!(l'_f - m'_f - 2K)!K!}, \quad (72)$$

$$M_{5f} = -A(m'_f=0)B(m'_f=0)iw_f d_1^{w_f-1} v^{l'_f-1} Y_{l'_f 0}^*(\hat{\nu}) \left[ 1 - \frac{b_1}{a_1} \right]^{\delta_f - l_f - k_f - i\nu_p} \\ \times {}_2F_1 \left[ l'_f + w_f - l_f - k_f + \delta_f, 1 - i\nu_p, l'_f + w_f + 1, \frac{b_1}{a_1} \right]. \quad (73)$$

The hypergeometric functions appearing in Eqs. (38), (41), (44)–(46), (67), (68), (70), (71), and (73) represent terminating series. Recently we have developed a similar technique<sup>20,36</sup> for the evaluation of these integrals in connection with electron capture from multielectron atoms in the continuum intermediate-state approximation.

### III. RESULTS AND DISCUSSIONS

The wave functions of the target atoms, helium and lithium may be expanded onto the basis of Slater-type orbitals with the help of Eqs. (10), (11), and (12). The Slater-orbital exponents<sup>9</sup> of the target atoms are presented

TABLE I. Description of orbitals of *s* symmetry of the target atoms.

Target atom	Basis	<i>s</i> orbital exponent	$\Phi(1s)$ expansion coefficients	$\Phi(2s)$ expansion coefficients
Orbital energy (a.u.)			-0.91795	
He 1s <sup>2</sup>	1s	1.417 14	0.768 38	
	1s	2.376 82	0.223 46	
	1s	4.396 28	0.040 82	
	1s	6.526 99	-0.009 94	
	1s	7.942 52	0.002 30	
Orbital energy			-2.477 73	-0.196 32
Li 1s <sup>2</sup> 2s <sup>1</sup>	1s	2.476 73	0.897 86	-0.146 29
	1s	4.698 73	0.111 31	-0.015 16
	2s	0.383 50	-0.000 08	0.003 77
	2s	0.660 55	0.001 12	0.980 53
	2s	1.070 00	-0.002 16	0.109 71
	2s	1.632 00	0.008 84	-0.110 21

ed in Table I.

In support of the present method we have calculated the  $J$  and  $K$  integrals in Eqs. (2) and (3) for a few low-lying bound states and compared the present computed results with those obtained by the help of parametric-differentiation technique. Identical results were found in both the methods for some particular values of the input parameter. We have also reproduced the results of Belkić, Gayet, and Salin<sup>8</sup> for the  $H^+ + Li$  collisions.

Calculations have been carried out at incident energies between 800 and 2500 keV for capture into all final states with  $n \leq 3$  for  $He^{2+} + Li(1s, 2s)$  collisions, between 200 keV/amu and 4 MeV/amu with  $n \leq 4$  for  $Li^{3+} + He(1s)$ , between 12 and 25.5 Mev with  $n \leq 5$  for  $C^{6+} + He(1s)$  and for  $O^{8+} + He(1s)$  collisions we have calculated our results at incident energies between 20 and 40 Mev for capture into all final states with  $n \leq 5$ . The present calculated total cross sections are displayed and compared with the existing theoretical results and available experimental findings.<sup>25-32</sup>

In Fig. 1 and Table II(a) and II(b) we present the  $K$ -shell,  $L$ -shell, and the total capture cross sections evaluated by applying the  $n^{-3}$  law for  $n \geq 3$ . The theoretical values are obtained from the relation

$$Q_{tot} = Q_{1s} + Q_{2s} + Q_{2p} + 2.081(Q_{3s} + Q_{3p} + Q_{3d}), \quad (74)$$

as the contributions from the higher excited states are

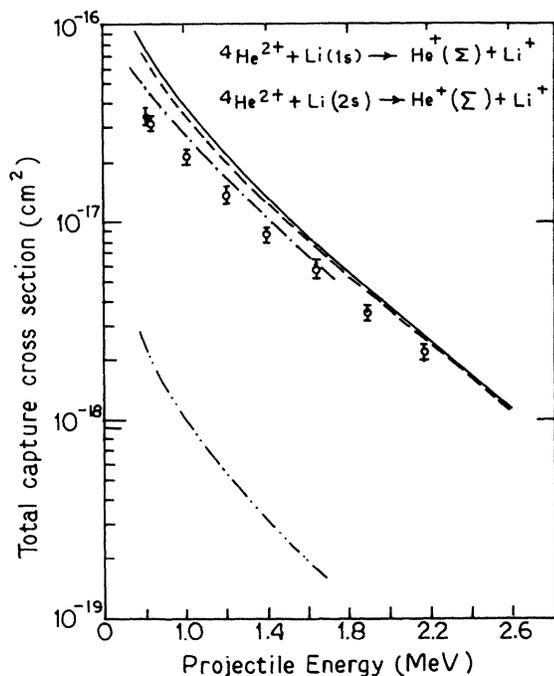


FIG. 1. Capture into all states by  $He^{2+}$  ions in lithium atoms. Theory: --- present results for capture from the  $K$  shell; — present results for capture from the  $L$ -shell; — present results for capture from all shells of  $He$ ; — CTMC calculation (Ref. 10). Experiments:  $\square$ , McCullough *et al.* (Ref. 32);  $\circ$ , Shah and Gilbody (Ref. 25).

TABLE II. The present CDW cross sections for charge transfer in (a)  $He^{2+} + Li(1s) \rightarrow He^+(\Sigma nl) + Li^+$  collisions and (b)  $He^{2+} + Li(2s) \rightarrow He^+(\Sigma nl) + Li^+$  collisions. (Numbers in square brackets denote the powers of ten by which the numbers are to be multiplied. The cross section of each subshell has been multiplied by two because either of the two electrons may be captured.)

Projectile energy (MeV)	$Q_{1s}$	$Q_{2s}$	$Q_{2p}$	$(Q_{2s} + Q_{2p})$	$Q_{3s}$	$Q_{3p}$	$Q_{3d}$	$(Q_{3s} + Q_{3p} + Q_{3d})$	$Q_{tot}$
0.8	4.87[-1]	7.80[-2]	2.56[-2]	1.03[-1]	2.90[-2]	1.38[-2]	8.50[-3]	5.13[-2]	6.96[-1]
1.0	2.52[-1]	4.10[-2]	1.38[-2]	5.48[-2]	1.53[-2]	6.46[-3]	3.65[-3]	2.54[-2]	3.58[-1]
1.25	1.26[-1]	2.10[-2]	6.60[-3]	2.76[-2]	7.60[-3]	2.90[-3]	1.48[-3]	1.19[-2]	1.78[-1]
1.5	6.94[-2]	1.16[-2]	3.61[-3]	1.52[-2]	4.0[-3]	1.46[-3]	6.86[-4]	6.14[-3]	9.73[-2]
2.0	2.54[-2]	4.22[-3]	1.20[-3]	5.42[-3]	1.44[-3]	4.65[-4]	1.88[-4]	2.09[-3]	3.51[-2]
2.5	1.10[-2]	1.81[-3]	4.70[-4]	2.28[-3]	6.0[-4]	1.81[-4]	6.56[-5]	8.46[-4]	1.50[-2]
0.8	1.10[-2]	2.92[-3]	2.80[-3]	5.72[-3]	1.59[-3]	8.06[-4]	7.95[-4]	3.19[-3]	2.33[-2]
1.0	5.59[-3]	1.36[-3]	10.99[-4]	2.45[-3]	6.56[-4]	3.25[-4]	2.77[-4]	12.57[-4]	1.06[-2]
1.25	2.69[-3]	6.02[-4]	4.14[-4]	10.16[-4]	2.61[-4]	12.65[-5]	9.40[-5]	4.81[-4]	4.70[-3]
1.5	1.42[-3]	2.99[-4]	1.82[-4]	4.81[-4]	1.21[-4]	5.71[-5]	3.81[-5]	2.16[-4]	2.35[-3]
2.5	2.04[-4]	3.67[-5]	1.62[-5]	5.29[-5]	1.29[-5]	5.42[-6]	2.90[-6]	2.12[-5]	3.01[-4]

found to be negligible. It is explicitly clear from Table II(a) and II(b) that the dominant contribution for single-electron capture comes from the final  $\text{He}^+(1s)$  state which is quite expected as the binding energy of the  $K$ -shell electron is near resonance with the final  $\text{He}^+(1s)$  state. At 800 keV,  $K$ -shell capture contribution from the core is about 97% of the total cross section and rises to 99% at 2500 keV, whereas  $L$ -shell electron capture cross section is only 3% at 800 keV and 1% at 2500 keV. We can, therefore, conclude that the single-electron capture process is primarily due to  $K$ -shell electron over most of the energy<sup>10,12</sup> range. We have also observed that the contribution for  $L$ -shell electron capture increases with the decrease in projectile energy. In Fig. 1, we compare our results with the CTMC<sup>10</sup> results in the intermediate energy region and with the experimental results of McCullough *et al.*<sup>32</sup> as well as of Shah and Gilbody.<sup>25</sup> In the intermediate energy region our results overestimate the CTMC results and the experimental findings of both McCullough *et al.*<sup>32</sup> and Shah and Gilbody,<sup>25</sup> while in the high-energy region the present calculated results are in good agreement with the observed findings.

In Fig. 2 and Table III the results for the  $\text{Li}^{3+} + \text{He}$

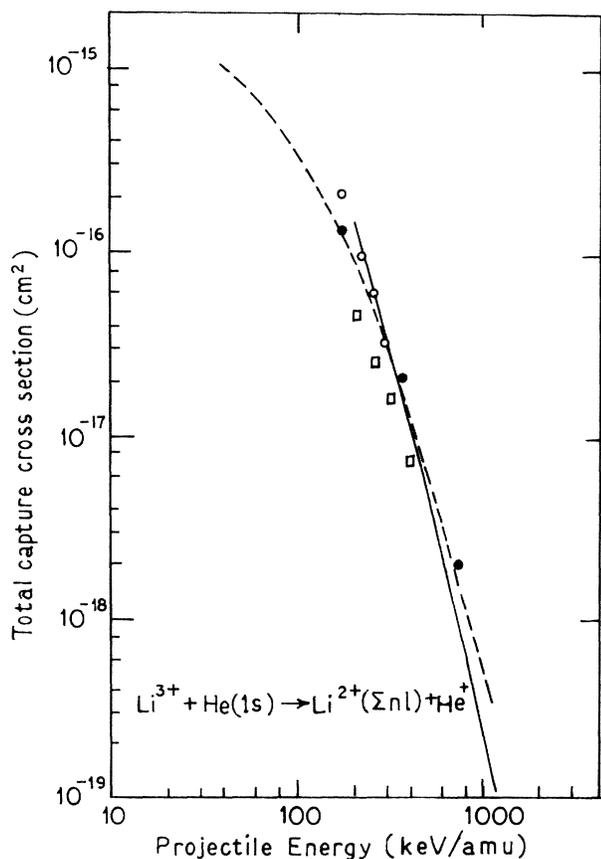


FIG. 2. Capture into all states by  $\text{Li}^{3+}$  ions in Helium atoms. Theory: —, present work; ---- UDWA calculations (Ref. 11). Experiments: ●, Nikolaev *et al.* (Ref. 27); ○, Pivovarov, Leuchen Kg, and Krivonosou (Ref. 28); □, Shah, Elliot, and Gilbody (Ref. 26).

TABLE III. The present CDW cross section for charge transfer in  $\text{Li}^{3+} + \text{He}(1s) \rightarrow \text{Li}^{2+}(\Sigma nl) + \text{He}^+$  collisions. (Numbers in square brackets denote the powers of ten by which the numbers are to be multiplied. The cross section of each subshell has been multiplied by two because either of the two electrons may be captured.) Total cross sections ( $10^{-16} \text{ cm}^2$ ).

Projectile energy (keV/amu)	$Q_{1s}$	$Q_{2s}$	$Q_{2p}$	$(Q_{2s} + Q_{2p})$	$Q_{3s}$	$Q_{3p}$	$Q_{3d}$	$(Q_{3s} + Q_{3p} + Q_{3d})$
200	2.0[-1]	1.20[-1]	2.19[-1]	3.39[-1]	1.27[-1]	7.40[-2]	7.96[-2]	2.80[-1]
300	7.96[-2]	3.50[-2]	4.56[-2]	8.06[-2]	2.60[-2]	1.43[-2]	1.35[-2]	5.38[-2]
500	1.80[-2]	5.68[-3]	5.0[-3]	1.06[-2]	2.98[-3]	1.54[-3]	1.10[-3]	5.62[-3]
700	5.64[-3]	1.48[-3]	1.02[-3]	2.50[-3]	6.60[-4]	3.27[-4]	1.83[-4]	1.17[-3]
800	3.44[-3]	8.46[-4]	5.30[-4]	1.37[-3]	3.56[-4]	1.72[-4]	8.80[-5]	6.16[-4]
1000	1.43[-3]	3.20[-4]	1.71[-4]	4.91[-4]	1.24[-4]	5.69[-5]	2.50[-5]	2.06[-4]
4000	2.39[-6]	3.64[-7]	7.89[-8]	4.43[-7]	1.13[-7]	2.89[-8]	4.28[-9]	1.46[-7]
	$Q_{4s}$	$Q_{4p}$	$Q_{4d}$	$Q_{4f}$	$(Q_{4s} + Q_{4p} + Q_{4d} + Q_{4f})$	$Q_{\text{tot}}$		
200	1.03[-1]	6.50[-2]	7.0[-2]	2.48[-2]	2.63[-1]	1.49[0]		
300	1.80[-2]	9.88[-3]	1.07[-2]	3.26[-3]	4.18[-2]	3.21[-1]		
500	1.72[-3]	8.65[-4]	7.85[-4]	2.13[-4]	3.58[-3]	4.34[-2]		
700	3.45[-4]	1.67[-4]	1.24[-4]	3.35[-5]	6.70[-4]	1.10[-2]		
800	1.80[-4]	8.63[-5]	5.83[-5]	1.59[-5]	3.41[-4]	6.30[-3]		
1000	6.04[-5]	2.78[-5]	1.61[-5]	4.62[-6]	1.09[-4]	2.41[-3]		
4000	4.90[-8]	1.34[-8]	4.37[-9]		6.67[-8]	3.14[-6]		

TABLE IV. The present CDW cross section for charge transfer in  $C^{6+} + He \rightarrow C^{5+}(\Sigma nl) + He^+$  collisions. (Numbers in square brackets denote the powers of ten by which the numbers are to be multiplied. The cross section of each subshell has been multiplied by two because either of the two electrons may be captured.) Total cross sections ( $10^{-16} \text{ cm}^2$ ). The contributions from  $Q_{3d}$ ,  $Q_{5f}$ , and  $Q_{5g}$  are found to be small in our calculations.

Projectile energy (MeV)	$Q_{1s}$	$Q_{2s}$	$Q_{2p}$	$(Q_{2s} + Q_{2p})$	$Q_{3s}$	$Q_{3p}$	$Q_{3d}$	$(Q_{3s} + Q_{3p} + Q_{3d})$
12	2.0[-3]	1.54[-3]	3.67[-3]	5.21[-3]	1.95[-3]	1.19[-3]	1.48[-3]	4.62[-3]
16	1.03[-3]	5.82[-4]	1.00[-3]	1.58[-3]	5.17[-4]	3.02[-4]	3.22[-4]	1.14[-3]
18.5	6.88[-4]	3.39[-4]	5.0[-4]	8.39[-4]	2.58[-4]	1.50[-4]	1.44[-4]	5.52[-4]
25.5	2.46[-4]	9.31[-5]	1.00[-4]	1.93[-4]	5.37[-5]	3.05[-5]	2.26[-5]	1.06[-4]
	$Q_{4s}$	$Q_{4p}$	$Q_{4d}$	$Q_{4f}$	$(Q_{4s} + Q_{4p} + Q_{4d} + Q_{4f})$	$Q_{5s}$	$Q_{5p}$	$(Q_{5s} + Q_{5p})$
12	1.69[-3]	8.75[-4]	1.06[-3]	3.07[-4]	3.94[-3]	1.31[-3]	7.42[-4]	2.05[-3]
16	3.80[-4]	1.82[-4]	2.25[-4]	5.51[-5]	8.43[-4]	2.68[-4]	1.37[-4]	4.05[-4]
18.5	1.77[-4]	8.42[-5]	9.92[-5]	2.27[-5]	3.83[-4]	1.20[-4]	5.94[-5]	1.79[-4]
25.5	3.19[-5]	1.54[-5]	1.51[-5]	3.26[-6]	6.58[-5]	1.99[-5]	9.81[-6]	2.97[-5]
	$Q_{6s}$	Experimental value (Dellingham <i>et al.</i> )						
12	1.99[-2]	$1.77 \pm 0.17[-2]$						
16	5.43[-3]	$5.72 \pm 0.39[-3]$						
18.5	2.83[-3]	$2.87 \pm 0.18[-3]$						
25.5	6.74[-4]	$8.39 \pm 0.75[-4]$						

collisions have been presented at incident energies between 200 keV/amu and 1 MeV/amu with  $n \leq 4$ . Calculations have been performed by applying the  $n^{-3}$  law for  $n \geq 4$  and are given by

$$Q_{\text{tot}} = Q_{1s} + Q_{2s} + Q_{2p} + Q_{3s} + Q_{3p} + Q_{3d} + 2.561(Q_{4s} + Q_{4p} + Q_{4d} + Q_{4f}), \quad (75)$$

as the contributions from the next-higher excited states are found to be small. We have compared the present calculated results with the theoretical UDWA results of Suzuki *et al.*<sup>11</sup> and with the experimental findings of Nikolaev *et al.*,<sup>27</sup> Pivovar, Leuchen Ko, and Krivonov,<sup>28</sup> and Shah, Elliot, and Gilbody.<sup>26</sup> We observe that above 200 keV/amu, our results are in satisfactory agreement with both the theoretical results of UDWA and the experimental findings, but slightly overestimates the results of Shah, Elliot, and Gilbody.<sup>26</sup> We have also noted that the major contribution for single-electron capture comes from the final Li<sup>2+</sup>(1s) state at and above 500 keV/amu. Our results for the total capture cross section at 4 MeV/amu (not shown in the figure) is  $3.14 \times 10^{-22}$  cm<sup>2</sup> which underestimates the theoretical values of Sidorovich, Nikolaev, and McGuire<sup>13</sup> calculated in the Bassel and Gerjuoy approximation<sup>14</sup> where they have not taken into account the contributions from the higher excited states. Unfortunately, no experimental result is available at this energy value to compare the theoretical methods.

In Fig. 3 and Table IV we present our calculated results for C<sup>6+</sup> + He collisions whereas in Fig. 4 and Table V we present the corresponding results for the O<sup>8+</sup> + He system. The theoretical results for the total cross section for the C<sup>6+</sup> + He collision have been calculated by applying the  $n^{-3}$  law for  $n \geq 5$ , which is given by

$$Q_{\text{tot}} = Q_{1s} + Q_{2s} + Q_{2p} + Q_{3s} + Q_{3p} + Q_{3d} + Q_{4s} + Q_{4p} + Q_{4d} + Q_{4f} + 2.047(Q_{5s} + Q_{5p} + Q_{5d} + Q_{5f} + Q_{5g}) \quad (76)$$

as the contributions from the higher excited states are found to be quite small in the total capture cross section. To justify the  $n^{-3}$  law we have also calculated the cross sections for  $n \geq 4$  and observed that the results obtained for  $n \geq 4$  and  $n \geq 5$  differ to the maximum extent of 9% up to 18.5 MeV and at 25.5 MeV the difference is within 5%. It should be clearly mentioned here that if one takes the higher values of  $n$ , the difference may, however, be minimized. But in our calculations, if we take higher values of  $n$ , the summations in Eq. (53) will lead to precisional error because of the occurrence of nearly equal terms with alternating signs. We have compared our calculated results with the experimental findings and observed that our results are in reasonably good agreement with the values of Dillingham, Macdonald, and Richard<sup>31</sup> in the energy region considered.

For O<sup>8+</sup> + He collision, calculations for the cross sections have been performed by applying the  $n^{-3}$  law for  $n \geq 5$  at incident energies between 20 and 40 MeV. The

TABLE V. The present CDW cross section for charge transfer in O<sup>8+</sup> + He → O<sup>7+</sup>(Σnl) + He<sup>+</sup> collisions. (Numbers in square brackets denote the powers of ten by which the numbers are to be multiplied. The cross section of each subshell has been multiplied by two because either of the two electrons may be captured.) Total cross sections (10<sup>-16</sup> cm<sup>2</sup>).

Projectile energy (MeV)	$Q_{1s}$	$Q_{2s}$	$Q_{2p}$	$(Q_{2s} + Q_{2p})$	$Q_{3s}$	$Q_{3p}$	$Q_{3d}$	$(Q_{3s} + Q_{3p} + Q_{3d})$
20	6.29[-4]	7.55[-4]	3.18[-3]	3.94[-3]	1.87[-3]	1.30[-3]	1.89[-3]	5.07[-3]
30	2.97[-4]	2.30[-4]	5.62[-4]	7.92[-4]	2.96[-4]	1.80[-4]	2.31[-4]	7.08[-4]
40	1.43[-4]	8.30[-5]	1.44[-4]	2.27[-4]	7.37[-5]	4.35[-5]	4.65[-5]	1.63[-4]
20	$Q_{4s}$	$Q_{4p}$	$Q_{4d}$	$(Q_{4s} + Q_{4p} + Q_{4d})$	$Q_{5s}$	$Q_{5p}$	$Q_{5d}$	$(Q_{5s} + Q_{5p} + Q_{5d})$
20	2.16[-3]	1.34[-3]	1.33[-3]	4.84[-3]	1.96[-3]	1.30[-3]	1.14[-3]	4.40[-3]
30	2.57[-4]	1.27[-4]	1.61[-4]	5.45[-4]	1.98[-4]	1.03[-4]	a	3.01[-4]
40	5.40[-5]	2.51[-5]	3.19[-5]	1.11[-4]	3.79[-5]	1.80[-5]	a	5.59[-5]
Experimental value (Dillingham <i>et al.</i> )								
20	$Q_{\text{tot}}$							
20	2.39[-2]							
30	1.63 ± 0.10[-2]							
30	2.89 ± 0.15[-3]							
40	7.59[-4]							
40	8.56 ± 1.02[-4]							

<sup>a</sup>The contributions from  $Q_{4f}$ ,  $Q_{5d}$ ,  $Q_{5f}$ , and  $Q_{5g}$  are found to be small in our calculations.

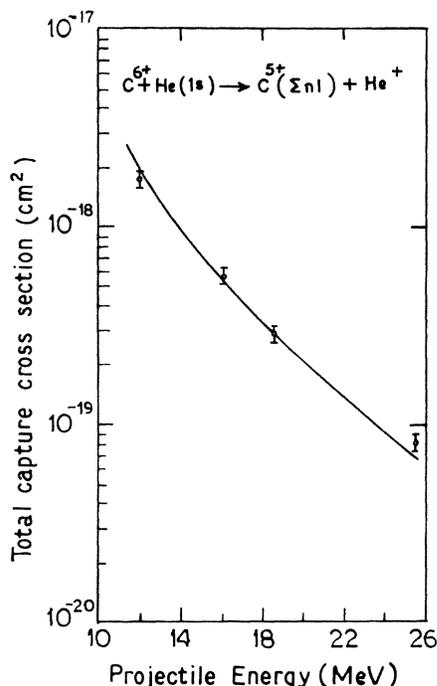


FIG. 3. Capture into all states by  $C^{6+}$  ions in helium atoms. Theory: —, present work. Experiment:  $\square$ , Dillingham, Macdonald, and Richard (Ref. 31).

cross sections thus obtained have also been compared with the cross sections obtained for  $n \geq 4$ . We have observed that the two results differ by about 7%. We have compared our calculated results with the existing experimental findings and observed that our results are in good agreement with the values of Dillingham, Macdonald, and

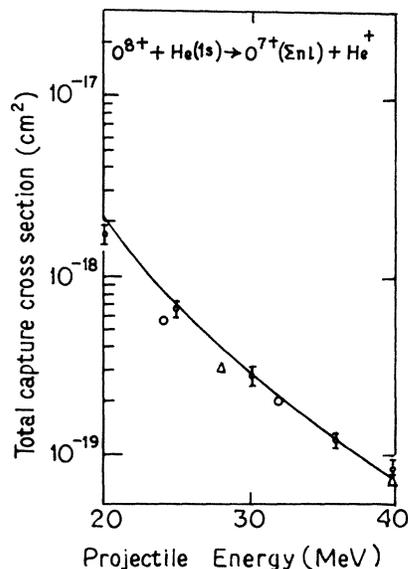


FIG. 4. Capture into all states by  $O^{8+}$  ions in helium atoms. Theory: —, present work. Experiments:  $\Delta$ , Macdonald and Martin (Ref. 29);  $\circ$ , Hippler *et al.* (Ref. 30);  $\square$ , Dillingham, Macdonald, and Richard (Ref. 31).

Richard<sup>31</sup> above 25 MeV, but overestimates slightly (Fig. 4) the values of Hippler *et al.*<sup>30</sup> and Macdonald and Martin<sup>29</sup> below 35 MeV. It is to be mentioned here that the experimental values are found to differ from one another through the energy region considered. Table V indicates that the contribution to the capture cross section from the  $n=3$  level is maximum. The theoretical results of CTMC and UDWA (not shown in Fig. 4) show fair agreement with our calculated results in the intermediate-energy region. Comparative study of Figs. 1–4 indicates that there is a uniform decrease in the values of the cross sections with the increase of incident projectile energy and also with the increase of the principal quantum number  $n$ .

#### IV. CONCLUSION

The present paper has been aimed at developing a generalized method for the evaluation of Coulomb integrals containing the product of the Coulomb wave function with Slater-type orbitals in a closed form in terms of the Gaussian hypergeometric function in a terminating series. The present method finds convenient numerical computation to obtain the charge-transfer cross section into arbitrary  $n$ ,  $l$ , and  $m$  states of the fast fully stripped projectiles from the multielectron atoms in the framework of the continuum distorted-wave approximation. We have obtained detailed theoretical predictions on single-electron capture cross sections for  $Li^{3+} + He$ ,  $O^{8+} + He$ ,  $C^{6+} + He$ , and  $He^{2+} + Li$  collisions which are found to be in good agreement with recent experimental data in the intermediate and high-energy region. In the present investigation we have used the active electron approximation ignoring the effect of the passive electrons as in the case of CDWA, SPBA, and other high-energy approximations. The experimental values, particularly in the case of the  $O^{8+} + He$  collisions, differ considerably between themselves throughout the energy region considered. Further experimental investigation and theoretical calculation by using a more realistic potential for the target may be suggested. In view of the success in predicting the cross sections for fully-stripped-ion–atom collisions in the intermediate- and high-energy region, this method may be helpful in connection with diagnostic techniques for studying the role played by the impurities in neutral-beam heating of fusion plasma.

#### ACKNOWLEDGMENTS

The authors acknowledge Professor N.C. Sil for his valuable suggestion and useful discussion. The authors would also like to express their thanks to the authorities of the Regional Computer Centre, Calcutta, for making available their Burroughs 6700 Computer in the course of this work. One of the authors (S.D.) acknowledges the University Grants Commission for their financial support. This work was supported in part by the International Atomic Energy Agency, Vienna, Austria, under Research Contract No. 3830/RB.

- <sup>1</sup>H. B. Gilbody, in *Advances in Atomic and Molecular Physics*, edited by D. R. Bates and B. Bederson (New York, Academic, 1979), Vol. 15, p. 293; *Applied Atomic Collision Physics*, edited by H. S. W. Massey, E. W. McDaniel, and B. Bederson (Academic Press, New York, 1984), Vol. 2.
- <sup>2</sup>B. H. Bransden and I. M. Cheshire, *Proc. Phys. Soc. London* **81**, 820 (1963).
- <sup>3</sup>J. P. Coleman and M. R. C. McDowell, *Proc. Phys. Soc. London* **85**, 1097 (1965).
- <sup>4</sup>J. P. Coleman, *Case Stud. At. Collision Phys.* **1**, 100 (1969).
- <sup>5</sup>I. M. Cheshire, *Proc. Phys. Soc. London* **84**, 89 (1964).
- <sup>6</sup>I. M. Cheshire, *Proc. Phys. Soc. London* **82**, 113 (1963); *Phys. Rev. A* **138**, 992 (1965).
- <sup>7</sup>R. Gayet, *J. Phys. B* **5**, 483 (1972).
- <sup>8</sup>Dž Belkić, R. Gayet, and A. Salin, *Phys. Rep.* **56**, 280 (1979).
- <sup>9</sup>E. Clemente and C. Roetti, *At. Data Nucl. Data Tables* **14**, 185 (1974).
- <sup>10</sup>R. E. Olson, *J. Phys. B* **15**, L163 (1982).
- <sup>11</sup>H. Suzuki, Y. Kajikawa, N. Toshima, T. Watanabe, and H. Ryufuku, *Phys. Rev. A* **29**, 525 (1984).
- <sup>12</sup>A. M. Ermolaev and B. H. Bransden, *Electronic and Atomic Collisions, Proceedings of the Thirteenth International Conference on the Physics of Electronic and Atomic Collisions, Berlin, 1983*, edited by J. Eichler, W. Fritsch, I. V. Hertel, N. Stolterfoht, and U. Wille (North-Holland, Amsterdam, 1983).
- <sup>13</sup>V. A. Sidorovich, V. S. Nikolaev, and J. H. McGuire, *Phys. Rev. A* **31**, 2193 (1985).
- <sup>14</sup>R. H. Bassel and F. Gerjuoy, *Phys. Rev.* **113**, 749 (1960).
- <sup>15</sup>J. Macek and S. Alston, *Phys. Rev. A* **26**, 250 (1982); S. Alston, *ibid.* **27**, 2342 (1983).
- <sup>16</sup>C. D. Lin, S. C. Soong, and L. N. Tunnell, *Phys. Rev. A* **17**, 1646 (1978).
- <sup>17</sup>J. S. Briggs, *Rep. Prog. Phys.* **39**, 217 (1976).
- <sup>18</sup>Mita Ghosh, C. R. Mandal, and S. C. Mukherjee, *J. Phys. B* **18**, 3797 (1985).
- <sup>19</sup>T. S. Ho, M. Lieber, F. T. Chan, and K. Omidvar, *Phys. Rev. A* **24**, 2933 (1981).
- <sup>20</sup>G. C. Saha, Shyamal Dutta, and S. C. Mukherjee, *Phys. Rev. A* **31**, 3633 (1985).
- <sup>21</sup>L. Kocbach, *J. Phys. B* **13**, L665 (1980).
- <sup>22</sup>Dž Belkić, *J. Phys. B* **17**, 3629 (1984).
- <sup>23</sup>Dž Belkić, *J. Phys. B* **14**, 1907 (1981); **16**, 2773 (1983).
- <sup>24</sup>L. J. Dubé, *J. Phys. B* **17**, 641 (1984).
- <sup>25</sup>M. B. Shah and H. B. Gilbody, *J. Phys. B* **18**, 899 (1985).
- <sup>26</sup>M. B. Shah, D. S. Elliot, and H. B. Gilbody, *J. Phys. B* **18**, 4245 (1985).
- <sup>27</sup>V. S. Nikolaev, I. S. Dmitriev, L. N. Fateeva, and Ya. A. Teplova, *Zh. Eksp. Teor. Fiz.* **40**, 989 (1961) [*Sov. Phys.—JETP* **13**, 695 (1961)].
- <sup>28</sup>L. I. Pivovarov, Yu. Z. Levchenko, and G. A. Krivonosov, *Zh. Eksp. Teor. Fiz.* **59**, 19 (1970) [*Sov. Phys.—JETP* **32**, 11 (1971)].
- <sup>29</sup>J. R. Macdonald and F. W. Martin, *Phys. Rev. A* **4**, 1965 (1971).
- <sup>30</sup>R. Hippler, S. Datz, P. D. Miller, and P. L. Pepmiller, in *Proceedings of the Fourteenth International Conference on the Physics of Electronic and Atomic Collisions, Palo Alto, 1985* edited by M. J. Coggiola, D. L. Huestis, R. P. Saxon (North-Holland, Amsterdam, 1985).
- <sup>31</sup>T. R. Dillingham, J. R. Macdonald, and P. Richard, *Phys. Rev. A* **24**, 1237 (1981).
- <sup>32</sup>R. W. McCullough, T. V. Goffe, M. B. Shah, M. Lennon, and H. B. Gilbody, *J. Phys. B* **15**, 111 (1982).
- <sup>33</sup>Dž Belkić, R. Gayet, and A. Salin, *Comput. Phys. Commun.* **30**, 193 (1983).
- <sup>34</sup>H. D. Todd, K. G. Kay, and H. J. Silverstone, *J. Chem. Phys.* **53**, 3951 (1970).
- <sup>35</sup>M. J. Caola, *J. Phys. A* **11**, L23 (1978).
- <sup>36</sup>Shyamal Datta, *J. Phys. B* **18**, 853 (1985).