# First-order theory for charge exchange with correct boundary conditions: General results for hydrogenlike and multielectron target atoms

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The first Born approximation of Belkić, Gayet, and Salin [Phys. Rep. **56**, 279 (1979)] with correct boundary conditions for charge exchange is thoroughly investigated. Functional analysis is used to derive general result $T^{(1)}_{nlm;n'l'm'}$ of the transition amplitude for electron capture from hydrogenlike and multielectron atoms by bare nuclei. The basic matrix element is a two-center Dalitz integral *with* the logarithmic Coulomb phase factors, which has a broad spectrum of applications in both atomic and molecular physics. Multielectron target atoms are treated within an independent-particle model which goes beyond the customary procedure for scaled hydrogenlike wave functions. An accurate and efficient algorithm is encoded for both hydrogenic and Roothaan-Hartree-Fock orbitals into a single program for charge exchange between completely stripped ions and arbitrary atoms. An exemplary computation of the total cross sections is presently carried out for electron capture from all shells of Li by $\alpha$ particles in the energy range from 250 to 2500 keV. Good agreement is found with recent experimental data of McCullough *et al.* [J. Phys. B **15**, 111 (1982)] and Sasao *et al.* [J. Phys. Soc. Jpn. **55**, 102 (1986)].

## I. INTRODUCTION

Standard scattering theory has originally been devised in nuclear physics, where interactions are of short range. These potentials leave the asymptotic channel states unaltered and, hence, the plane wave is commonly used to describe the relative motion of the heavy particles.[1-3] Such a formalism has customarily been extended to atomic physics without the essential modifications. However, atomic-collision processes involve long-range Coulomb potentials which are, in general, present even when the scattering particles are at infinite separation from each other. This peculiarity causes distortion of unperturbed channel states which, in turn, yields some modifications of the perturbation potentials. These two major components of scattering theory are interrelated and cannot be arbitrarily changed, i.e., any change in the Coulomb phase of the wave functions will induce a change in the perturbing potential.[4] Hence, the usual scattering theory must be reformulated whenever long-range Coulomb potentials are present in the asymptotic region. This is the boundary-condition problem which requires that both initial- and final-state wave functions exhibit correct asymptotic behavior at infinite internuclear separation $R$. This is equivalent to the asymptotic convergence problem[4] which consists of showing an existing of Møller wave matrices $\Omega^{(+)}$ and $\Omega^{(-)}$. Ignoring this problem, as has repeatedly been done in the literature,[5,6] will imply divergence of the scattering operator $S$ as well as other related quantities of physical interest, such as the transition amplitude $T$, etc. This conclusion has been reached by Dollard[4] with mathematical rigor, for both potential scattering and the multichannel problem.

The fundamental work of Dollard,[4] however, did not receive due attention for a long time and, hence, its relevance was limited to only formal aspects of Coulomb scattering. It has been only recently[7] that a consistent procedure was proposed along the lines of Dollard's study and within the most basic rearrangement collisions of heavy particles. In their derivation of an exact eikonal $T$ matrix, Belkić *et al.*[7] have imposed the correct boundary conditions to both channel states. As a result, the exact $T$ matrix possesses the following three important properties. (i) Perturbation potentials $W_i$ and $W_f$ causing the transition are of short range as $R \to \infty$ through all orders in the $T$ operator ($T = W_f + W_f G_e^+ W_i$). (ii) The total eikonal Green's function $G_e^+$, as well as potentials $W_i$ and $W_f$ do not contain internuclear interaction $V_\gamma(R)$. (iii) Stationary channel states $\Phi_i^+$ and $\Phi_f^-$ occurring in the exact $T$ matrix exhibit logarithmic Coulomb phase distortion. These phase factors are dependent upon $R$, but do not bear any relationship with the internuclear potential $V_\gamma(R)$ and must be retained in the computation of both differential as well as *total* cross sections.

The most important consequence of these properties is that the *exact* eikonal $T$ matrix of Belkić *et al.*[7] is free from the singularities which have originally been revealed by Dollard,[4] Mapleton,[5] and Carpenter and Tuan[6] and rediscovered more recently by Dewangan and Eichler[8] (see also Ref. 9).

The present work is concerned with the first-order approximation to the exact eikonal $T$ matrix of Ref. 7. Previous results[10,11] which have been obtained by means of this conceptually plausible scattering theory were encouraging and have motivated us to carry out an extensive analytical study of the most general transition amplitude for charge exchange in collisions between fast bare nuclei and hydrogenlike as well as multielectron atoms. As an illustration, detailed numerical computations have been performed for electron capture from the $K$ and $L$ shell of

 

a lithium atom by $\alpha$ particles. Atomic units will be used throughout the work unless stated otherwise.

## II. THEORY

Consider charge exchange of the prototype

$$Z_P+(Z_T,e)_i\rightarrow(Z_P,e)_f+Z_T\ , \tag{2.1}$$

where $Z_P$ and $Z_T$ are the nuclear charges of the projectile and target. Indices $i$ and $f$ are the collective labels for the usual set of quantum numbers $n^i l^i m^i$ and $n^f l^f m^f$, respectively. Let $\mathbf{r}_P$ and $\mathbf{r}_T$ be the position vectors of the electron relative to $Z_P$ and $Z_T$, respectively. Further, let $\mathbf{R}$ be the position vector of $Z_T$ with respect to $Z_P$.

The "prior" and the "post" forms of the transition amplitude for process (2.1), in the first Born approximation with asymptotically correct boundary conditions, can be written as follows:[7]

$$T_{if}^{(-)}(\boldsymbol{\eta})=\int\int d\mathbf{r}_i d\mathbf{r}_T \varphi_f^{Z_P*}(\mathbf{r}_P)\left[\frac{Z_P}{R}-\frac{Z_P}{r_P}\right]\times\varphi_i^{Z_T}(\mathbf{r}_T)e^{i\mathbf{k}_i\cdot\mathbf{r}_i+i\mathbf{k}_f\cdot\mathbf{r}_f}\mathscr{E}(\mathbf{R})\ , \tag{2.2a}$$

$$T_{if}^{(+)}(\boldsymbol{\eta})=\int\int d\mathbf{r}_f d\mathbf{r}_P \varphi_f^{Z_P*}(\mathbf{r}_P)\left[\frac{Z_T}{R}-\frac{Z_T}{r_T}\right]\times\varphi_i^{Z_T}(\mathbf{r}_T)e^{i\mathbf{k}_i\cdot\mathbf{r}_i+i\mathbf{k}_f\cdot\mathbf{r}_f}\mathscr{E}(\mathbf{R})\ , \tag{2.2b}$$

where $\boldsymbol{\eta}$ is the transverse momentum transfer, and

$$\mathscr{E}(\mathbf{R})=\exp\left[i\frac{Z_P(Z_T-1)}{v}\ln(vR-\mathbf{v}\cdot\mathbf{R})+i\frac{Z_T(Z_P-1)}{v}\ln(vR+\mathbf{v}\cdot\mathbf{R})\right]\ . \tag{2.3}$$

Here, $\varphi_i^{Z_T}(\mathbf{r}_T)$ and $\varphi_f^{Z_P}(\mathbf{r}_P)$ are the initial and final bound-state wave functions, $\mathbf{v}$ is the incident velocity vector, $\mathbf{k}_i$ and $\mathbf{k}_f$ are the initial and final momenta. Further, $\mathbf{r}_i$ ($\mathbf{r}_f$) is the position vector of the center of mass of system $Z_T-e$ ($Z_P-e$) relative to $Z_P$ ($Z_T$), respectively.

Whenever the initial and final bound states are exactly known, as in the case of hydrogenlike atoms, the prior and the post transition amplitudes yield the same result. Nevertheless, for the purpose of a straightforward generalization of the present method to multielectron atoms, for which there is a post-prior discrepancy, we shall hereafter calculate simultaneously $T_{if}^{(-)}(\boldsymbol{\eta})$ and $T_{if}^{(+)}(\boldsymbol{\eta})$.

Calculation of transition amplitudes (2.2a) and (2.2b) is possible with the most general form of auxiliary function $\mathscr{E}(\mathbf{R})$ containing the two exponential factors with the Coulomb phases. As a result, the one-dimensional integrals over nonterminating Gauss hypergeometric functions ${}_2F_1$ would be encountered. This is, however, unnecessary since Eq. (2.3) can readily be simplified as follows:

$$\mathscr{E}(\mathbf{R})=(\rho v)^{2iZ_P(Z_T-1)/v}\exp[-i\xi\ln(vR+\mathbf{v}\cdot\mathbf{R})]\ , \tag{2.4a}$$

$$\mathscr{E}(\mathbf{R})=(\rho v)^{2iZ_T(Z_P-1)/v}\exp[+i\xi\ln(vR-\mathbf{v}\cdot\mathbf{R})]\ , \tag{2.4b}$$

where $\xi=(Z_T-Z_P)/v$ and $\rho$ is the impact parameter ($\mathbf{R}=\boldsymbol{\rho}+\mathbf{Z}$, $\boldsymbol{\rho}\cdot\mathbf{Z}=0$). Multiplying terms $(\rho v)^{2iZ_P(Z_T-1)/v}$ and $(\rho v)^{2iZ_P(Z_T-1)/v}$ do not contribute to the total cross section and, therefore, the single Coulomb phase such as $\exp[-i\xi\ln(vR+\mathbf{v}\cdot\mathbf{R})]$ or $\exp[+i\xi\ln(vR-\mathbf{v}\cdot\mathbf{R})]$ need to be retained in the calculation. Hence, the phase factor $(\rho v)^{2iZ_P(Z_T-1)/v}$ or $(\rho v)^{2iZ_T(Z_P-1)/v}$ can freely be dropped from the transition amplitudes and we are finally led to

$$T_{if}^{(-)}(\boldsymbol{\eta})=\int\int d\mathbf{r}_i d\mathbf{r}_T \varphi_f^{Z_P*}(\mathbf{r}_P)\left[\frac{Z_P}{R}-\frac{Z_P}{r_P}\right]\varphi_i^{Z_T}(\mathbf{r}_T)\times e^{i\mathbf{k}_i\cdot\mathbf{r}_i+i\mathbf{k}_f\cdot\mathbf{r}_f-i\xi\ln(vR+\mathbf{v}\cdot\mathbf{R})}\ , \tag{2.5a}$$

$$T_{if}^{(+)}(\boldsymbol{\eta})=\int\int d\mathbf{r}_f d\mathbf{r}_P \varphi_f^{Z_P*}(\mathbf{r}_P)\left[\frac{Z_T}{R}-\frac{Z_T}{r_T}\right]\varphi_i^{Z_T}(\mathbf{r}_T)\times e^{i\mathbf{k}_i\cdot\mathbf{r}_i+i\mathbf{k}_f\cdot\mathbf{r}_f-i\xi\ln(vR+\mathbf{v}\cdot\mathbf{R})}\ . \tag{2.5b}$$

As to the differential cross section, however, phase factor $(\rho v)^{2iZ_P(Z_T-1)/v}$ or $(\rho v)^{2iZ_T(Z_P-1)/v}$ plays an essential role.[12,13] Hence, in the most general case with $Z_P\neq1\neq Z_T$, quantities $T_{if}^{(-)}$ and $T_{if}^{(+)}$ derived respectively from Eqs. (2.5a) and (2.5b) will not be proportional to the differential cross section. Nevertheless, Eqs. (2.5a) and (2.5b) can still be used for the purpose of computing $d\sigma_{if}^{(1)}/d\Omega$, provided that the missing phase $(\rho v)^{2iZ_P(Z_T-1)/v}$ is subsequently accounted for, via

$$\frac{d\sigma_{if}^{(\pm)}}{d\Omega}=\left|\mu v\int d\boldsymbol{\rho}\,\rho^{2iZ_P(Z_T-1)/v}\mathscr{A}_{if}^{(\pm)}(\boldsymbol{\rho})\right|^2\left[\frac{a_0^2}{\text{sr atom}}\right]\ , \tag{2.6}$$

where $\mathscr{A}_{if}^{(\pm)}(\boldsymbol{\rho})$ are the impact-parameter-dependent transition amplitudes which can be obtained by taking the Fourier transforms of quantities (2.5a) and (2.5b), respectively.[7] Hence, for every practical purpose of computing the total as well as the differential cross sections, formulas (2.5a) and (2.5b) with the single Coulomb phase $\exp[-i\xi\ln(vR+\mathbf{v}\cdot\mathbf{R})]$ can be used.

Introducing the Fourier transform $f(\mathbf{q})$ by

$$f(\mathbf{q})=(2\pi)^{-3}\int d\mathbf{r}\,e^{i\mathbf{q}\cdot\mathbf{r}}f(\mathbf{r}) \tag{2.7}$$

we obtain the following result from Eqs. (2.5a) and (2.5b):

$$T_{if}^{(-)}(\boldsymbol{\eta})=Z_P I_{if;0}^{(0,0)}(\boldsymbol{\eta})-\tfrac{1}{2}I_{if;1}^{(0,-1)}(\boldsymbol{\eta})\ , \tag{2.8a}$$

$$T_{if}^{(+)}(\boldsymbol{\eta})=Z_T I_{if;0}^{(0,0)}(\boldsymbol{\eta})-\tfrac{1}{2}I_{if;1}^{(-1,0)}(\boldsymbol{\eta})\ , \tag{2.8b}$$

where $I_{if;\sigma}^{(\nu_i,\nu_f)}(\boldsymbol{\eta})$ is an auxiliary integral of the type

$$I_{if;\sigma}^{(\nu_i,\nu_f)}(\boldsymbol{\eta})=(2\pi)^{-3}\int d\mathbf{R}\,R^{\sigma-1}(vR+\mathbf{v}\cdot\mathbf{R})^{-i\xi}\int d\mathbf{q}\,e^{-i\mathbf{q}\cdot\mathbf{R}}\frac{\tilde{\varphi}_f^{Z_P*}(\mathbf{q}-\boldsymbol{\alpha})\tilde{\varphi}_i^{Z_T}(\mathbf{q}+\boldsymbol{\beta})}{(|\mathbf{q}-\boldsymbol{\alpha}|^2+\alpha_f^2)^{\nu_f}(|\mathbf{q}+\boldsymbol{\beta}|^2+b_f^2)^{\nu_i}} \tag{2.9}$$

with

$$\boldsymbol{\alpha}=\boldsymbol{\eta}+\alpha_z\hat{\mathbf{v}},\quad \boldsymbol{\beta}=-\boldsymbol{\eta}+\beta_z\hat{\mathbf{v}},\quad \boldsymbol{\eta}=(\eta\cos\phi_\eta,\eta\sin\phi_\eta,0)$$

$$\alpha_z=\frac{\Delta E}{v}-\frac{v}{2},\quad \beta_z=-\frac{\Delta E}{v}-\frac{v}{2},$$

$$\Delta E=E_i-E_f=-\frac{b_i^2}{2}+\frac{a_f^2}{2} \tag{2.10}$$

$$a_f=Z_P/n^f,\quad b_i=Z_T/n^i,\quad \boldsymbol{\alpha}+\boldsymbol{\beta}=\mathbf{v}\ .$$

The hydrogenlike wave function in the momentum space is given by

$$\tilde{\varphi}_j^{Z_K}(\mathbf{q})=(2\pi)^{-3}N_j^{Z_K}i^{l^j}\times\sum_{p_j=0}^{n_r^j}c_{p_j}\frac{\mathscr{Y}_{l^jm^j}(\mathbf{q})}{[q^2+(Z_K/n^j)^2]^{p_j+l^j+2}}, \tag{2.11}$$

where $\mathscr{Y}_{lm}(\mathbf{q})=q^lY_{lm}(\hat{\mathbf{q}})$,

$$N_j^{Z_K}=16\pi Z_K\left[\frac{(Z_K/n^j)^3}{n^j}\frac{(n^j+l^j)!}{n_r^j!}\right]^{1/2}\frac{l^j!(4Z_K/n^j)^{l^j}}{(2l^j+1)!},$$

$$c_{p_j}=\frac{(-n_r^j)_{p_j}(n^j+l^j+1)_{p_j}}{(l^j+\frac{3}{2})_{p_j}p_j!}\left[\frac{Z_K}{n^j}\right]^{p_j}, \tag{2.12}$$

$$(a)_k=\Gamma(a+k)/\Gamma(a),\quad n_r^j=n^j-l^j-1$$

$$(j=i,\ f;K=P,T)\ .$$

Hence,

$$I_{if;\sigma}^{(\nu_i,\nu_f)}(\boldsymbol{\eta})=i^{l^i}(-i)^{l^f}N_i^{Z_T}N_f^{Z_P}\sum_{p_i=0}^{n_r^i}\sum_{p_f=0}^{n_r^f}c_{p_i}c_{p_f}H_{n_in_f;\sigma}^{(\nu_i,\nu_f)}(\boldsymbol{\alpha},\boldsymbol{\beta}), \tag{2.13a}$$

$$H_{n_in_f;\sigma}^{(\nu_i,\nu_f)}(\boldsymbol{\alpha},\boldsymbol{\beta})=2\pi^2\mathscr{H}_{n_in_f;\sigma}^{(\nu_i,\nu_f)}(\boldsymbol{\alpha},\boldsymbol{\beta}), \tag{2.13b}$$

where

$$\mathscr{H}_{n_in_f;\sigma}^{(\nu_i,\nu_f)}(\boldsymbol{\alpha},\boldsymbol{\beta})=(2\pi)^{-3}\int d\mathbf{R}\,R^{\sigma-1}(vR+\mathbf{v}\cdot\mathbf{R})^{-i\xi}\times\mathscr{G}_{n_in_f}^{\nu_i\nu_f}(-\mathbf{R}), \tag{2.14}$$

$$\mathscr{G}_{n_in_f}^{\nu_i\nu_f}(\mathbf{R})=\frac{1}{2\pi^2}\int d\mathbf{q}\,e^{i\mathbf{q}\cdot\mathbf{R}}\times\frac{\mathscr{Y}_{l^fm^f}^*(\mathbf{q}-\boldsymbol{\alpha})\mathscr{Y}_{l^im^i}(\mathbf{q}+\boldsymbol{\beta})}{(|\mathbf{q}-\boldsymbol{\alpha}|^2+a_f^2)^{n_f+1}(|\mathbf{q}+\boldsymbol{\beta}|^2+b_i^2)^{n_i+1}} \tag{2.15}$$

with $n_j=p_j+l^j+\nu_j+1$ $(j=i,f)$.

### A. Calculation of integral $\mathscr{G}$

Using the Feynman identity[14]

$$\frac{1}{A^nB^m}=\frac{(n+m-1)!}{(n-1)!(m-1)!}\times\int_0^1 dt\,t^{n-1}(1-t)^{m-1}[At+B(1-t)]^{-n-m}$$

$$(n,m\geq 1) \tag{2.16}$$

we can write

$$\mathscr{G}_{n_in_f}^{\nu_i\nu_f}(\mathbf{R})=\frac{n!}{n_i!n_f!}\int_0^1 dt\,t^{n_f}(1-t)^{n_i}U_{n_in_f}^{\nu_i\nu_f}(\mathbf{R}), \tag{2.17}$$

where

$$U_{n_in_f}^{\nu_i\nu_f}(\mathbf{R})=\frac{e^{i\mathbf{Q}\cdot\mathbf{R}}}{2\pi^2}\int d\mathbf{q}\,e^{i\mathbf{q}\cdot\mathbf{R}}\frac{\mathscr{Y}_{l^fm^f}^*(\mathbf{q}+\mathbf{Q}_\alpha)\mathscr{Y}_{l^im^i}(\mathbf{q}+\mathbf{Q}_\beta)}{(q^2+\Delta^2)^{n+1}} \tag{2.18}$$

with

$$\mathbf{Q}=\boldsymbol{\alpha}t-\boldsymbol{\beta}(1-t),\quad \Delta^2=v^2t(1-t)+a_f^2t+b_i^2(1-t),$$
$$\mathbf{Q}_\alpha=\mathbf{Q}-\boldsymbol{\alpha}=(1-t)\mathbf{v},\quad \mathbf{Q}_\beta=\mathbf{Q}+\boldsymbol{\beta}=-t\mathbf{v}, \tag{2.19}$$
$$n=n_i+n_f+1\ .$$

Next, by employing an addition and recombination formula for the regular solid harmonic $\mathscr{Y}_m(\mathbf{q})$ we shall have[15]

$$\mathscr{Y}_{l^fm^f}^*(\mathbf{q}+\mathbf{Q}_\alpha)\mathscr{Y}_{l^im^i}(\mathbf{q}+\mathbf{Q}_\beta)=\sum_{l_1^i=0}^{l^i}\sum_{l_1^f=0}^{l^f}\sum_{m_1^i=-l_1^i}^{+l_1^i}\sum_{m_1^f=-l_1^f}^{+l_1^f}\sum_{l=l^{if}}^{\lambda}{}^{(2)}t^{l_2^i}(1-t)^{l_2^f}\Omega_{l_1^im_1^i}^{l_1^fm_1^f}(l,\mathbf{v})q^{\lambda-l}\mathscr{Y}_{lm}(\mathbf{q}), \tag{2.20}$$

where

$$\Omega_{l_1^im_1^i}^{l_1^fm_1^f}(l,\mathbf{v})=(l_1^im_1^i\,|\,l^im^i)(l_1^fm_1^f\,|\,l^fm^f)\langle l_1^im_1^i\,|\,l_1^fm_1^f\,|\,lm\rangle\mathscr{Y}_{l_2^fm_2^f}^*(\mathbf{v})\mathscr{Y}_{l_2^im_2^i}(-\mathbf{v}), \tag{2.21a}$$

$$(l_1^j m_1^j \mid l^j m^j)=\left[4\pi\frac{2l^j+1}{(2l_1^j+1)(2l_2^j+1)}\frac{(l^j+m^j)!}{(l_1^j+m_1^j)!(l_2^j+m_2^j)!}\frac{(l^j-m^j)!}{(l_1^j-m_1^j)!(l_2^j-m_2^j)!}\right]^{1/2}, \tag{2.21b}$$

$$\langle l_1^i m_1^i \mid l_1^f m_1^f \mid lm\rangle=(-1)^{m_1^i}\left[\frac{(2l_1^i+1)(2l_1^f+1)(2l+1)}{4\pi}\right]^{1/2}\begin{bmatrix} l_1^f & l_1^i & l \\ 0 & 0 & 0\end{bmatrix}\begin{bmatrix} l_1^f & l_1^i & l \\ -m_1^f & m_1^i & -m\end{bmatrix}, \tag{2.21c}$$

$$l_1^j+l_2^j=l^j,\quad m_1^j+m_2^j=m^j,\quad -l_2^j\le m_2^j\le +l_2^j,\quad m=m_1^i-m_1^f,\quad \lambda=l_1^i+l_1^f, \tag{2.21d}$$

and

$$l^{if}=\begin{cases}\max(\,|l_1^i-l_1^f|,|m|\,) & \text{if } \max(\,|l_1^i-l_1^f|,|m|\,)+\lambda \text{ even},\\ \max(\,|l_1^i-l_1^f|,|m|\,)+1 & \text{if } \max(\,|l_1^i-l_1^f|,|m|\,)+\lambda \text{ odd}.\end{cases} \tag{2.21e}$$

Here, quantity $\langle l_1^i m_1^i \mid l_1^f m_1^f \mid lm\rangle$ represents the Gaunt coefficient and

$$\begin{bmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3\end{bmatrix}$$

is the Wigner $3j$ symbol.[16] The upper index (2) in Eq. (2.20), associated with symbol $\sum^{(2)}$, indicates that the summation is to be carried out in steps of two, due to the parity coefficient $\left(\begin{smallmatrix} l_1^f & l_1^i & l \\ 0 & 0 & 0\end{smallmatrix}\right)$, which is equal to zero unless $\lambda+l$ is even.[16] Thus, we can write

$$U_{n_i n_f}^{\nu_i \nu_f}(\mathbf{R})=e^{i\mathbf{Q}\cdot\mathbf{R}}\sum_{l_1^i=0}^{l^i}\sum_{l_1^f=0}^{l^f}\sum_{m_1^i=-l_1^i}^{+l_1^i}\sum_{m_1^f=-l_1^f}^{+l_1^f}\sum_{l=l^{if}}^{\lambda}{}^{(2)}t^{l_2^i}(1-t)^{l_2^f}\Omega_{l_1^i m_1^i}^{l_1^f m_1^f}(l,\mathbf{v})W_{n_i n_f}^{\nu_i \nu_f}(\mathbf{R}), \tag{2.22}$$

with

$$W_{n_i n_f}^{\nu_i \nu_f}(\mathbf{R})=\frac{1}{2\pi^2}\int d\mathbf{q}\, e^{i\mathbf{q}\cdot\mathbf{R}}\frac{q^{\lambda-l}\mathscr{Y}_{lm}(\mathbf{q})}{(q^2+\Delta^2)^{n+1}}. \tag{2.23}$$

Angular integrations over $\Omega_{\mathbf{q}}=(\theta_{\mathbf{q}},\phi_{\mathbf{q}})$ in Eq. (2.23) can be carried out by means of the partial-wave expansion of the plane wave, i.e.,

$$\exp(i\mathbf{q}\cdot\mathbf{R})=4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{+l} i^l j_l(qR)Y_{lm}^*(\hat{\mathbf{q}})Y_{lm}(\hat{\mathbf{R}}), \tag{2.24}$$

where $j_l(z)$ is the spherical Bessel function. This implies

$$W_{n_i n_f}^{\nu_i \nu_f}(\mathbf{R})=i^l F_{nl}^{\lambda}(R)\mathscr{Y}_{lm}(\mathbf{R}), \tag{2.25}$$

where

$$F_{nl}^{\lambda}(R)=\frac{2}{\pi R^l}\int_0^{\infty} dq\frac{q^{\lambda+2}j_l(qR)}{(q^2+\Delta^2)^{n+1}}. \tag{2.26}$$

The result of the radial integral (2.26) is given by[15]

$$F_{nl}^{\lambda}(R)=(-1)^{\lambda_l}\frac{\Delta^{(\lambda+l)-2n+1}}{2^n n!}\times\sum_{s=0}^{\lambda_l}(-n)_s(-\lambda_l)_s\hat{k}_{\nu-1/2}(R\Delta)\frac{(-2)^s}{s!}, \tag{2.27}$$

where $\lambda_l=(\lambda-l)/2<n$, $\nu=n-s-l$, and $\hat{k}_{\mu}(z)$ is the reduced Bessel function[17]

$$\hat{k}_{\mu}(z)=\sqrt{2/\pi}z^{\mu}K_{\mu}(z), \tag{2.28}$$

with $K_{\mu}(z)$ being the McDonald function [Gradshteyn and Ryzhik,[18] Eq. (8.468)]. Hence,

$$U_{n_i n_f}^{\nu_i \nu_f}(\mathbf{R})=\frac{e^{i\mathbf{Q}\cdot\mathbf{R}}}{2^n n!}\sum_{l_1^i=0}^{l^i}\sum_{l_1^f=0}^{l^f}\sum_{m_1^i=-l_1^i}^{+l_1^i}\sum_{m_1^f=-l_1^f}^{+l_1^f}\sum_{l=l^{if}}^{\lambda}{}^{(2)}i^l(-1)^{\lambda_l}t^{l_2^i}(1-t)^{l_2^f}\Omega_{l_1^i m_1^i}^{l_1^f m_1^f}(l,\mathbf{v})\frac{\mathscr{S}_{nlm}^{(\Delta)}(\mathbf{R})}{\Delta^{2n-(\lambda+l)-1}}, \tag{2.29}$$

and

$$\mathscr{S}_{nlm}^{(\Delta)}(\mathbf{R})=\sum_{s=0}^{\lambda_l}(-n)_s(-\lambda_l)_s B_{vlm}^{(\Delta)}(\mathbf{R})\frac{(-2)^s}{s!}, \tag{2.30}$$

where $B_{vlm}^{(\Delta)}(\mathbf{R})$ is the so-called $B$ function of Filter and Steinborn,[17]

$$B_{vlm}^{(\Delta)}(\mathbf{R})=\hat{k}_{\nu-1/2}(R\Delta)\mathscr{Y}_{lm}(\mathbf{R}). \tag{2.31}$$

The final form of integral $\mathscr{G}$ is, therefore, reduced to

$$\mathscr{G}^{\nu_i\nu_f}_{n_i n_f}(\mathbf{R})=\frac{e^{i\mathbf{Q}\cdot\mathbf{R}}}{n_i!n_f!2^n}\sum_{l_1^i=0}^{l^i}\sum_{l_1^f=0}^{l^f}\sum_{m_1^i=-l_1^i}^{+l_1^i}\sum_{m_1^f=-l_1^f}^{+l_1^f}\sum_{l=l^{if}}^{\lambda}{}^{(2)}\, i^l(-1)^{\lambda_l}\Omega^{l_1^f m_1^f}_{l_1^i m_1^i}(l,\mathbf{v})\int_0^1 dt\, t^{n_f+l_2^i}(1-t)^{n_i+l_2^f}\frac{\mathscr{S}^{(\Delta)}_{nlm}(\mathbf{R})}{\Delta^{2n-(\lambda+l)-1}}\ . \tag{2.32}$$

### B. Calculation of integral $\mathscr{H}$

Inserting result (2.32) into Eq. (2.14) we deduce

$$\mathscr{H}^{(\nu_i,\nu_f)}_{n_i n_f;\sigma}(\boldsymbol{\alpha},\boldsymbol{\beta})=\frac{1/2}{n_i!n_f!}\sum_{l_1^i=0}^{l^i}\sum_{l_1^f=0}^{l^f}\sum_{m_1^i=-l_1^i}^{+l_1^i}\sum_{m_1^f=-l_1^f}^{+l_1^f}\sum_{l=l^{if}}^{\lambda}{}^{(2)}(-1)^{\lambda_l}i^l\Omega^{l_1^f m_1^f}_{l_1^i m_1^i}(l,\mathbf{v})\mathscr{I}^{(\sigma)}_{nlm}\ , \tag{2.33}$$

with

$$\mathscr{I}^{(\sigma)}_{nlm}=\int_0^1 dt\, t^{n_f+l_2^i}(1-t)^{n_i+l_2^f}\frac{\tilde{\mathscr{S}}^{(\sigma,\Delta)}_{nlm}(\mathbf{Q})}{\Delta^{2n-(\lambda+l)-1}}\ , \tag{2.34}$$

where

$$\tilde{\mathscr{S}}^{(\sigma,\Delta)}_{nlm}(\mathbf{Q})=\sum_{s=0}^{\lambda_l}(-n)_s(-\lambda_l)_s\tilde{B}^{(\sigma,\Delta)}_{\nu lm}(\mathbf{Q})\frac{(-2)^s}{s!}\ . \tag{2.35}$$

Here $\tilde{B}^{(\sigma,\Delta)}_{\nu lm}(\mathbf{Q})$ is the Fourier transform of function $B^{(\sigma,\Delta)}_{\nu lm}(\mathbf{R})$ introduced by

$$B^{(\sigma,\Delta)}_{\nu lm}(\mathbf{R})=R^{\sigma-1}(vR-\mathbf{v}\cdot\mathbf{R})^{-i\xi}B^{(\Delta)}_{\nu lm}(\mathbf{R})\ . \tag{2.36}$$

The general result for integrals of this type is obtained in Appendix A, from which it follows

$$\frac{1}{2^{n-1}}\tilde{\mathscr{S}}^{(\sigma,\Delta)}_{nlm}(\mathbf{Q})=\frac{i^l}{2\pi^2}L^{(\sigma,\Delta)}_{nlm}(\mathbf{Q})\ , \tag{2.37}$$

where

$$L^{(\sigma,\Delta)}_{nlm}(\mathbf{Q})=\frac{(2n_r)!}{n_r!}\sum_{p=0}^{n_r}\frac{(-n_r)_p}{(-2n_r)_p}\,{}_3F_2\left[-n,-\lambda_l,-n_r+p;-n_r+\frac{p}{2},-n_r+\frac{p+1}{2};1\right]G^{(\sigma,\Delta)}_{\bar{p}lm}(\mathbf{Q},\mathbf{v})\frac{2^{p-2n_r}\Delta^p}{p!}\ , \tag{2.38}$$

with

$$G^{(\sigma,\Delta)}_{\bar{p}lm}(\mathbf{Q},\mathbf{v})=\sum_{\kappa=0}^{p_\sigma}\sum_{l_1=0}^{l}\mathscr{I}^{\kappa l l_1}_{pl}(\sigma)D^{l_1}_{lm}(\mathbf{Q},\mathbf{v})\ , \tag{2.39}$$

$$\mathscr{I}^{\kappa l l_1}_{pl}(\sigma)=ab\,{}_3F_2\left[-\frac{\kappa_\sigma}{2},-\frac{\kappa_\sigma-1}{2},1-i\gamma_1;\kappa+l+1,-p_\sigma-l;\frac{\Delta^2+Q^2}{\Delta^2}\right]\ , \tag{2.40}$$

$$D^{l_1}_{lm}(\mathbf{Q},\mathbf{v})=\sum_{m_1=-l_1}^{+l_1}(l_1m_1\,|\,lm)\mathscr{Y}_{l_1m_1}(\mathbf{Q})\mathscr{Y}_{l_2m_2}(-i\mathbf{v})\ , \tag{2.41}$$

and

$$a=\Gamma(1-i\xi)(l+1)_{p_\sigma}\frac{(2\Delta)^{p_\sigma}}{(\Delta^2+Q^2)^{p_\sigma+l+1}}\ , \tag{2.42a}$$

$$b=\frac{(1-\xi)_{l_1}(i\xi)_{l_2}}{x^{i\gamma_2}}\frac{(-p_\sigma)_\kappa(i\gamma_2)_\kappa}{(l+1)_\kappa}\frac{(1-y/x)^\kappa}{\kappa!}\ , \tag{2.42b}$$

$$(l_1m_1\,|\,lm)=\left[4\pi\frac{2l+1}{(2l_1+1)(2l_2+1)}\frac{(l+m)!}{(l_1+m_1)!(l_2+m_2)!}\frac{(l-m)!}{(l_1-m_1)!(l_2-m_2)!}\right]^{1/2}\ , \tag{2.42c}$$

$$x=\frac{2}{Q^2+\Delta^2}(v\Delta-i\mathbf{Q}\cdot\mathbf{v})\ , \tag{2.42d}$$

$$y=v/\Delta\ , \tag{2.42e}$$

$$l_1+l_2=l,\quad m_1+m_2=m,\quad -l_2\le m_2\le+l_2\ , \tag{2.42f}$$

$$n_r=n-l-1,\quad \kappa_\sigma=p_\sigma-\kappa,\quad p_\sigma=p+\sigma \tag{2.42g}$$

$$\gamma_1=\xi+il_1,\quad \gamma_2=\xi-il_2\ . \tag{2.42h}$$

Here, ${}_3F_2$'s are the Claussen generalized hypergeometric polynomials[19]

$${}_3F_2\left[-n,-\lambda_l,-n_r+p;-n_r+\frac{p}{2},-n_r+\frac{p+1}{2};1\right]=\sum_{s=0}^{\min(\lambda_l,n_r-p)}\frac{(-n)_s(-\lambda_l)_s(-n_r+p)_s}{\left[-n_r+\frac{p}{2}\right]_s\left[-n_r+\frac{p+1}{2}\right]_s}\frac{1}{s!}\ , \tag{2.43a}$$

$${}_3F_2\left[-\frac{\kappa_\sigma}{2},-\frac{\kappa_\sigma-1}{2},1-i\gamma_1;\kappa+l+1,-p_\sigma-l;\frac{\Delta^2+Q^2}{\Delta^2}\right]=\sum_{u=0}^{\left[\frac{\kappa_\sigma}{2}\right]}\frac{(-\kappa_\sigma/2)_u(-\kappa_\sigma+\frac{1}{2})_u(1-i\gamma_1)_u}{(\kappa+l+1)_u(-p_\sigma-l)_u u!}\left[\frac{\Delta^2+Q^2}{\Delta^2}\right]^u, \tag{2.43b}$$

where $[\kappa_\sigma/2]$ is an integral part of $\kappa_\sigma/2$. Finally, we can infer that

$$\begin{aligned}H^{(\nu_i,\nu_f)}_{n_i n_f;\sigma}(\boldsymbol{\alpha},\boldsymbol{\beta})=&\frac{1}{n_i!n_f!}\sum_{l_1^i=0}^{l^i}\sum_{l_1^f=0}^{l^f}\sum_{m_1^i=-l_1^i}^{+l_1^i}\sum_{m_1^f=-l_1^f}^{+l_1^f}\sum_{l=l^{if}}^{\lambda}{}^{(2)}(-1)^{(\lambda+l)/2}\frac{(2n_r)!}{(n_r)!}\Omega^{l_1^f m_1^f}_{l_1^i m_1^i}(l,\mathbf{v})\\&\times\sum_{p=0}^{n_r}\frac{(-n_r)_p}{(-2n_r)_p}\,{}_3F_2\left[-n,-\lambda_l,-n_r+p;-n_r+\frac{p}{2},-n_r+\frac{p+1}{2};1\right]\frac{2^{p-2n_r-1}}{p!}\\&\times\int_0^1 dt\,t^{n_f+l_2^i}(1-t)^{n_i+l_2^f}\frac{G^{(\sigma,\Delta)}_{\bar{p}lm}(\mathbf{Q},\mathbf{v})}{\Delta^{2n-(\lambda+l)-p-1}}\ .\end{aligned} \tag{2.44}$$

### C. Choice of the quantization axis

The most general result (2.44) is valid for any axis of quantization of the hydrogenlike wave functions involved. However, considerable simplifications arise if we choose the quantization axis of both initial and final bound-state wave functions along the same vector $\mathbf{v}$. Thus with choice $\hat{\mathbf{v}}=(0,0,1)$, we shall have

$$\Omega^{l_1^f m_1^f}_{l_1^i m_1^i}(l,\mathbf{v})=\Omega^{lm}_{l_1^i l_1^f}(\mathbf{v})\delta_{m_2^i,0}\delta_{m_2^f,0}\ , \tag{2.45}$$

where $\delta_{i,j}$ is the usual Kronecker $\delta$ symbol, and

$$\begin{aligned}\Omega^{lm}_{l_1^i l_1^f}(\mathbf{v})=&(l_1^i\mid l^i m^i)(l_1^f\mid l^f m^f)\langle l_1^i m^i\mid l_1^f m^f\mid lm\rangle\\&\times v^{l_2^f}(-v)^{l_2^i}\quad (m=m^i-m^f)\ ,\end{aligned} \tag{2.46}$$

$$(l_1^j\mid l^j m^j)=\left\{\frac{2l^j+1}{2l_1^j+1}\frac{(l^j+m^j)!}{(l_1^j+m^j)!l_2^j!}\times\frac{(l^j-m^j)!}{(l_1^j-m_1^j)!l_2^j!}\right\}^{1/2}. \tag{2.47}$$

We can write, in general, $\mathbf{Q}=\boldsymbol{\alpha}+(1-t)\mathbf{v}=-\boldsymbol{\beta}-t\mathbf{v}$, from which it follows that for $\mathbf{v}=(0,0,v)$, azimuthal angle $\phi_Q$ of vector $\mathbf{Q}$ becomes independent of integration variable $t$, i.e., $\phi_Q=\phi_\alpha=\phi_\beta-\pi(\phi_\alpha\overset{*}{=}\phi_\eta)$. This implies

$$D^{l_1}_{lm}(\mathbf{Q},\mathbf{v})=\hat{D}^{l_1}_{lm}(\mathbf{Q}\cdot\mathbf{v})\Phi_m(\phi_\eta)\ , \tag{2.48}$$

where

$$\hat{D}^{l_1}_{lm}(\mathbf{Q}\cdot\mathbf{v})=(l_1\mid lm)(-iv)^{l_2}Q^{l_1}\mathscr{P}_{l_1 m}(\mathbf{Q}\cdot\hat{\mathbf{v}})\ , \tag{2.49}$$

with $\mathscr{P}_{l_1 m}$ being the normalized Legendre function of the first kind,

$$\begin{aligned}\mathscr{P}_{l_1 m}(z)=&(-1)^m\left[\frac{2l_1+1}{2}\frac{(l_1-m)!}{(l_1+m)!}\right]^{1/2}\\&\times(1-z^2)^{m/2}\left[\frac{d}{dz}\right]^{l_1+m}\frac{(z^2-1)^{l_1}}{2^{l_1}l_1!}\qquad(m\geq 0)\end{aligned} \tag{2.50a}$$

$$\mathscr{P}_{l_1,-m}(z)=(-1)^m\mathscr{P}_{l_1 m}(z)\ , \tag{2.50b}$$

$$\Phi_m(\phi_\eta)=(2\pi)^{-1/2}\exp(im\phi_\eta)\ . \tag{2.50c}$$

Hence, general result (2.44) is simplified as follows, for $\hat{\mathbf{v}}\|\hat{\mathbf{Z}}$:

$$H^{(\nu_i,\nu_f)}_{n_i n_f;\sigma}(\boldsymbol{\alpha},\boldsymbol{\beta})=\hat{H}^{(\nu_i,\nu_f)}_{n_i n_f;\sigma}(\boldsymbol{\alpha}\cdot\mathbf{v},\boldsymbol{\beta}\cdot\mathbf{v})\Phi^*_{m^f}(\phi_\alpha)\Phi_{m^i}(\phi_\beta)\ , \tag{2.51}$$

with $\hat{H}^{(\nu_i,\nu_f)}_{n_i n_f;\sigma}(\boldsymbol{\alpha}\cdot\mathbf{v},\boldsymbol{\beta}\cdot\mathbf{v})$ being independent of azimuthal angles $\phi_\alpha,\phi_\beta$ and

$$\left[\frac{2}{\pi}\right]^{1/2}\hat{H}_{n_i n_f;\sigma}^{(\nu_i,\nu_f)}(\boldsymbol{\alpha}\cdot\mathbf{v},\boldsymbol{\beta}\cdot\mathbf{v})=\frac{1}{n_i!n_f!}\sum_{l_1^i=|m^i|}^{l^i}\sum_{l_1^f=|m^f|}^{l^f}\sum_{l=l^{if}}^{\lambda}{}^{(2)}(-1)^{(\lambda+l)/2-m^i}\frac{(2n_r)!}{(n_r)!}\Omega_{l_1^i l_1^f}^{lm}(\mathbf{v})$$
$$\times\sum_{p=0}^{n_r}\frac{(-n_r)_p}{(-2n_r)_p}\,{}_3F_2\left[-n,-\lambda_l,-n_r+p;-n_r+\frac{p}{2},-n_r+\frac{p+1}{2};1\right]\frac{2^{p-2n_r}}{p!}$$
$$\times\int_0^1 dt\,t^{n_f+l_2^i}(1-t)^{n_i+l_2^f}\frac{g_{\bar{p}lm}^{(\sigma,\Delta)}(\mathbf{Q}\cdot\mathbf{v})}{\Delta^{2n-(\lambda+l)-p-1}}\,, \tag{2.52}$$

where

$$g_{\bar{p}lm}^{(\sigma,\Delta)}(\mathbf{Q}\cdot\mathbf{v})=\sum_{\kappa=0}^{p_\sigma}\sum_{l_1=|m|}^{l}\mathscr{I}_{pl}^{\kappa l_1}(\sigma)\hat{D}_{lm}^{l_1}(\mathbf{Q}\cdot\mathbf{v})\,. \tag{2.53}$$

Upon inserting final result (2.51) into Eqs. (2.13a) and (2.13b), auxiliary integral (2.9) is completed. Therefore, the resulting transition amplitudes (2.8a) and (2.8b) can be calculated in the most general case in terms of a one-dimensional real integral. This conclusively proves that the first Born approximation with correct boundary conditions in both scattering channels can be computed as efficiently as the approach of Jackson and Schiff (see Belkić and Taylor[15]).

Henceforth, choice $\hat{\mathbf{v}}=(0,0,1)$ will be understood, and this is particularly advantageous while calculating the eikonal total cross section defined by

$$\sigma_{if}^{(1)}(a_0^2)=\int_0^\infty d\eta\,\eta\int_0^{2\pi}d\phi_\eta\left|\frac{T_{if}^{(1)}(\eta)}{2\pi v}\right|^2, \tag{2.54}$$

where $T_{if}^{(1)}(\eta)$ is either $T_{if}^{(-)}$ or $T_{if}^{(+)}$. Integration over azimuthal angle $\phi_\eta$ can be performed analytically due to the factored dependence (2.51) of the integrand in Eq. (2.54). The remaining integral over $\eta$ must be performed numerically and this is best accomplished through the scaling of quadrature points towards the dominating forward cone by means of a suitable change of variable, such as

$$z=(\eta^2-2)/(\eta^2+2)\,. \tag{2.55}$$

where $z\in[-1,+1]$. Details about an explicit and regular form of transition amplitude $T_{if}^{(1)}(z)$ as a function of new variable $z$ can be found in Ref. 20.

The above analysis can readily be extended to collisions involving multielectron targets, such as

$$Z_P+(Z_T,e;\{e_1,e_2,e_3,\ldots,e_N\})_i$$
$$\rightarrow(Z_P,e)_f+(Z_T;\{e_1,e_2,e_3,\ldots,e_N\})_{i'}\,, \tag{2.56}$$

where set $\{e_1,e_2,e_3,\ldots,e_N\}$ represents the noncaptured electrons and the remaining notation is analogous to that for reaction (2.1). In applying the present theory to process (2.56) we shall devise an essentially one-electron model which is based upon the following assumptions.[7] (i) All of $N$ noncaptured electrons are considered as "passive" in the sense that the correlation effects are neglected, i.e., the interaction potentials between the active electron and the passive ones are weak and do not contribute to charge transfer. Furthermore, in this picture the passive electrons occupy the same orbitals before and after the collision. (ii) The perturbation potentials occurring in the prior $W_i$ $(=Z_P/R-Z_P/r_P)$ and post $W_f$ $(=Z_T^{\rm eff}/R-Z_T^{\rm eff}/r_T)$ forms of the transition amplitude are of short range as $R\rightarrow\infty$. Here $\mathbf{r}_{P,T}$ are the active electron coordinates with the same meaning as in process (2.1) and $Z_T^{\rm eff}$ is an effective charge to be conveniently chosen. It is consistent, within this model, to neglect the post collisional state of target rest $(Z_T;\{e_1,e_2,e_3,\ldots,e_N\})_{i'}$ in the exit channel.

Assumptions (i) and (ii) reduce process (2.56) to a one-electron problem (2.1) with $Z_T=Z_T^{\rm eff}$. The multielectron nature of the target, however, is present through initial-state wave function $\varphi_i^{Z_T^{\rm eff}}(\mathbf{r}_T)$ which we shall choose to be the Roothaan-Hartree-Fock (RHF) orbital as computed by Clementi and Roetti.[21] It is *within this model* that we impose the correct boundary conditions to both of the channel asymptotic states which are consistent with the above potentials $W_i$ and $W_f$. This will lead again to prior and post transition amplitudes (2.2a), (2.2b), (2.5a), and (2.5b) with $Z_T=Z_T^{\rm eff}$, $\xi=(Z_T^{\rm eff}-Z_P)/v$ and $E_i=\varepsilon_i$ where $\varepsilon_i$ is the Roothaan-Hartree-Fock orbital energy obtained variationally in Ref. 21. Finally, we shall choose effective charge $Z_T^{\rm eff}$ to be in the form proposed by Belkić *et al.*,[7] i.e., $Z_T^{\rm eff}=[-2(n^i)^2\varepsilon_i]^{1/2}$ where $n^i$ is the principal quantum number of the orbital occupied by the active electron to be captured.

Unlike process (2.1), this time we need to compute both prior and post forms of the transition amplitude since they are unequal and, furthermore, there is no firm theoretical ground upon which either of them should be favored. Hence, we have decided to introduce an average transition amplitude $T_{if}^{(1)}$ in the following symmetrical form:

$$T_{if}^{(1)}(\eta)=\tfrac{1}{2}[T_{if}^{(-)}(\eta)+T_{if}^{(+)}(\eta)]\,, \tag{2.57}$$

where $T_{if}^{(-)}$ and $T_{if}^{(+)}$ are defined by Eqs. (2.2a) and (2.2b) or (2.5a) and (2.5b) with $Z_T=Z_T^{\rm eff}$, $\xi=(Z_T^{\rm eff}-Z_P)/v$ $E_i=\varepsilon_i$ and with $\varphi_i^{Z_T^{\rm eff}}(\mathbf{r}_T)$ being the RHF orbital.[21] The Fourier transform of RHF wave function $\varphi_i^{Z_T^{\rm eff}}(\mathbf{r}_T)$ can be expressed as a linear combination of momentum-space-normalized Slater-type orbitals which have recently been obtained in the form of Gegenbauer polynomials by Belkić.[22] This has enabled us to extend the analysis for hydro-

genlike atoms to multielectron targets. Appropriate changes in the evaluation of matrix elements, however, are required. For example, Eq. (2.8b) has been derived using the following eigenvalue problem: $(\frac{1}{2}\nabla^2_{\mathbf{r}_T}+Z_T/r_T+E_i)\varphi_i^{Z_T}(\mathbf{r}_T)=0$. This equation ceases to be valid for the RHF orbital $\varphi_i^{Z_T^{\rm eff}}(\mathbf{r}_T)$ and, therefore, the matrix element with potential $-Z_T^{\rm eff}/r_T$ must be computed in a slightly different manner. Nevertheless, the basic mathematical apparatus is very much similar to the one following Eqs. (2.8a) and (2.8b) and need not be reiterated.

## III. ALGORITHMS

We have devised an algorithm into a single program for both hydrogenlike and multielectron target atoms in the most general case of arbitrary initial and final quantum numbers. The axis of quantization for initial and final bound states has been chosen along the same vector of incident velocity $\mathbf{v}$, which enormously simplified the angular-momentum algebra. The present version of the program is primarily concerned with the total cross section for electron capture from any target atom by bare nuclei. Differential cross sections for the case when either $Z_P$ or $Z_T$ are equal to unity are also available from our program. A more general problem with arbitrary nuclear charges requires special consideration in evaluation of cross sections $d\sigma_{if}^{(1)}/d\Omega$ and this is deferred to a future publication.

A number of test runs have been carried out in order to check the accuracy and efficiency of the algorithm. The present algorithm reproduces exactly the results of Belkić and Taylor[15] for the so-called two-center Dalitz integral. Furthermore, it has been verified in the case of arbitrary nuclear charges that the partial differentiation technique for all the possible combinations between $n^i l^i m^i$ and $n^f l^f m^f$ with $n^i \leq 3$ and $n^f \leq 3$ is in exact agreement with our general program for both hydrogenic and RHF orbitals. A detailed account of a more thorough test can be found in Ref. 20, where it has been seen that the present algorithm is capable of efficiently providing results with any prescribed degree of accuracy.

## IV. RESULTS AND COMPARISON WITH EXPERIMENTAL DATA

Our general program has already been used in a number of exhaustive computations of differential and total cross sections for electron capture from hydrogen-atom and multielectron targets by bare nuclei. Collisions of type $H^+$-H and $H^+$-Ar have been investigated in Ref. 11. A remarkable improvement of the present theory over the standard first Born approximation of Jackson and Schiff[23] has been achieved by using a simple hydrogenic model for Ar. Nevertheless, it would be desirable to employ a more realistic description of multielectron atoms, such as the present RHF model.

Recently, Belkić *et al.*[24] have studied reaction (2.1) with projectile charge $Z_P$ ranging from 1 to 6 and for a fixed $Z_T=1$. Excellent agreement has been obtained between the present theory and experimental data in contrast to the usual Jackson-Schiff[23] approximation, which largely overestimates the measurement. The findings of Ref. 24 are very important since they have clearly established a role of the boundary-condition problem in the framework of the first-order theories. This has been done within a purely hydrogenic problem in both channels of reaction (2.1), which is of a particular relevance for theoretical models due to the availability of the exact bound-state wave functions. Nevertheless, in order to make a general and full assessment about the validity of the theory in regard to experiment, it would be of considerable interest to perform a systematic study of capture processes in multielectron atoms.

In this section we shall be concerned with electron capture into any state of $He^+$ by fast $\alpha$ particles from a lithium atom, i.e.,

$$^4He^{2+}+Li(1s^2,2s^1)\rightarrow {}^4He^+(\Sigma)+Li^+ . \tag{4.1}$$

An independent-particle model of Sec. II will be adopted for this reaction with the RHF orbital for the ground state of lithium.[21] Experimental data of McCullough *et al.*[25] and Sasao *et al.*[26] relate to total cross sections for electron capture from all shells of Li into any state of $He^+$. Hence, we have computed cross sections for each $K$ and $L$ shell independently and their combined result $\sigma_{K+L}^{(1)}(\Sigma_4)$ was compared with the measurements, i.e.,

$$\sigma_{K+L}^{(1)}(\Sigma_4)=2\sigma_K^{(1)}(\Sigma_4)+\sigma_L^{(1)}(\Sigma_4) . \tag{4.2}$$

Total cross sections for electron capture from an individual shell of Li by an $\alpha$ particle into any state ($\Sigma$) of $He^+$ has been computed by means of Eq. (2.54) with scaled integration variable (2.55) and average transition amplitude $T_{if}^{(1)}$ given by Eq. (2.57). We shall henceforth use the following abbreviations:

$$\sigma_{if}^{(1)}=\sigma_{i;f}^{(1)}\equiv\sigma_{i;n^f l^f m^f}^{(1)} , \tag{4.3a}$$

$$\sigma_{i;n^f l^f}^{(1)}=\sum_{m^f=-l^f}^{+l^f}\sigma_{i;n^f l^f m^f}^{(1)} , \tag{4.3b}$$

$$\sigma_{i;n^f}^{(1)}=\sum_{l^f=0}^{n^f-1}\sigma_{i;n^f l^f}^{(1)} , \tag{4.3c}$$

$$\sigma_i^{(1)}(\Sigma)=\sum_{n^f=1}^{\infty}\sigma_{i;n^f}^{(1)} . \tag{4.3d}$$

In practice, the infinite summation in (4.3d) has been truncated and the scaling $(n^f)^{-3}$ law was used to make an estimate of the type[11]

$$\sigma_i^{(1)}(\Sigma)\simeq\sigma_i^{(1)}(\Sigma_N)\equiv\sum_{n^f=1}^{N}\sigma_{i;n^f}^{(1)}+\gamma(3,N)\sigma_{i;N+1}^{(1)} , \tag{4.4}$$

where

$$\gamma(3,N)=1+(N+1)^3\zeta(3)-\sum_{n^f=1}^{N+1}\left[\frac{N+1}{n^f}\right]^3 , \tag{4.5}$$

with $\zeta(3)$ being the Riemann zeta function.[27] By setting the upper limit to be equal to 4 we shall be investigating the convergence of the following sequence: $\sigma_i^{(1)}(\Sigma_1)$, $\sigma_i^{(1)}(\Sigma_2)$, $\sigma_i^{(1)}(\Sigma_3)$, and $\sigma_i^{(1)}(\Sigma_4)$, i.e.,

$$\sigma_i^{(1)}(\Sigma_1)=1.202\sigma_{i;1}^{(1)}\ , \tag{4.6a}$$

$$\sigma_i^{(1)}(\Sigma_2)=\sigma_{i;1}^{(1)}+1.616\sigma_{i;2}^{(1)}\ , \tag{4.6b}$$

$$\sigma_i^{(1)}(\Sigma_3)=\sigma_{i;1}^{(1)}+\sigma_{i;2}^{(1)}+2.081\sigma_{i;3}^{(1)}\ , \tag{4.6c}$$

$$\sigma_i^{(1)}(\Sigma_4)=\sigma_{i;1}^{(1)}+\sigma_{i;2}^{(1)}+\sigma_{i;3}^{(1)}+3.113\sigma_{i;4}^{(1)}\ . \tag{4.6d}$$

Cross sections (4.3a)—(4.3d) for capture of an electron from the $K$ shell of Li are respectively listed in Tables I(a)—I(d). It can be observed from Table I(c) that the $n^f=1$ level of $He^+$ yields the dominant contribution throughout the energy range under consideration, i.e., $E=250$—2500 keV. The Roothaan-Hartree-Fock orbital energy[21] for the $K$ shell is $\varepsilon_i=-2.477\,73$, which yields the following value for the effective charge:

$$Z_T^{\rm eff}=(-2\varepsilon_i)^{1/2}=2.226\,086\ (K\ \text{shell})\ . \tag{4.7}$$

This value of $Z_T^{\rm eff}$ is close to the projectile charge $Z_P=2$, and hence transition $\alpha+\mathrm{Li}(K\ \text{shell})\rightarrow\mathrm{He}^+(1s)+\mathrm{Li}^+$ is of a nearly resonant nature, within the present model. An inspection of Table I(d) will reveal that the convergence rate of sequence (4.6a)—(4.6d) is extremely good.

Corresponding results for cross sections (4.3a)—(4.3d) relating to capture from the $L$ shell of Li are presented in Tables II(a)—II(d), respectively. This time, at energies $E\lesssim 1500$ keV, electron capture into excited states of $He^+$ plays an important role. It can be seen from Table II(d), that at the lower edge, $E=250$ keV, the largest contribution to the $L$-shell capture comes from the $n^f=3$ level of $He^+$. The $L$-shell RHF orbital energy[21] of Li is $\varepsilon_i=-0.196\,320$, which implies

$$Z_T^{\rm eff}=(-8\varepsilon_i)^{1/2}=1.253\,220\ (L\ \text{shell})\ . \tag{4.8}$$

On the other hand, the electronic binding energy of $He^+(n^f=3)$ is $E_f=-0.222\,222$, which is very close to the RHF orbital energy $\varepsilon_i=-0.196\,320$, and therefore the reaction path $\alpha+\mathrm{Li}(L\ \text{shell})\rightarrow\mathrm{He}^+(n^f=3)+\mathrm{Li}^+$ provides a near-resonant contribution. Notice that although the excited states are very important for the $L$-shell capture, the size $N=4$ of sequence (4.6a)—(4.6d) is satisfactory in obtaining a good convergence at higher energies [see Table II(d)].

Total cross sections summed over all the initial and final states are displayed in Table III, from which it follows that capture from the $K$ shell of Li dominates the corresponding contribution from the target $L$ shell. The situation is, however, reversed at energies lower than those presented in this work.

Comparison between the present theory and measurements is depicted in Fig. 1, where satisfactory agreement is obtained. Also displayed on this figure are the results of the continuum-distorted-wave approximation as computed by Ghosh *et al.*[28] It is quite surprising that this higher-order theory, which is supposed to be adequate[7] for process (4.1) at energies greater than roughly 800 keV, fails to reproduce experimental data.

Results of the classical trajectory Monte Carlo method obtained by Olson[29] (not shown on Fig. 1) are found to be in very good agreement with our cross sections. It has previously been observed by Shipsey *et al.*[30] as well as by Bransden and Ermolaev[31] that at energies below 100 keV, capture from a Li atom by $\alpha$ particles into the $n^f=3$ level of $He^+$ gives the major contribution. This excited state of $He^+$ will subsequently decay to its ground $1s$ level either directly or by cascades via intermediate allowed transitions emitting soft-x-ray photons. An inverted level distribution of final states can be produced in this way, which is required for laser action in the far-ultraviolet or soft-x-ray region. In their analysis of double electron capture, Post *et al.*[32] have proposed the use of a neutral lithium atom beam to probe the $\alpha$-particle distribution in tokamak fusion reactors. The present results for energies $E\gtrsim 250$ keV show that the ground state of $He^+(1s)$ yields the main contribution to the total cross sections in $\alpha$-Li ($K$-shell) collisions. Hence, reaction (4.1) can hardly be used at these energies for the production of soft-x-ray lasers.

Charge exchange of types (2.1) and (2.56) find their applications in various areas such as plasma physics, astrophysics, etc. When the target is atomic hydrogen in its ground state and the projectile is a stripped metallic multiple ion, electron transfer (2.1) appears to be one of the

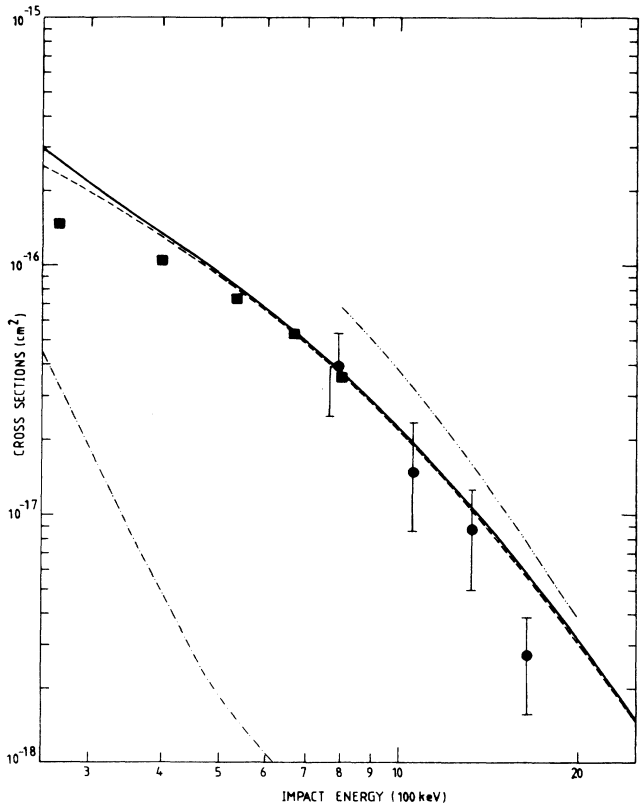


FIG. 1. Total capture cross sections $\sigma_i^{(1)}(\Sigma_4)$ in cm$^2$ for charge-exchange reaction (4.1) as a function of laboratory impact energy $E$ (keV). Index $i$ refers to the $K$, $L$, or $(K+L)$ shells. The results relating to electron transfer from an individual shell of Li are obtained by means of Eq. (4.6d), whereas $\sigma_{K+L}^{(1)}(\Sigma_4)$ is computed by means of Eq. (4.2). Theory: Present results: (—·—·—·, $L$ shell; — — —, $K$ shell; and ——, $(K+L)$ shells). The continuum-distorted-wave approximation: —··—··—···—, Ghosh *et al.* (Ref. 28). Experimental data: ■, McCullough *et al.* (Ref. 25) and ●, Sasao *et al.* (Ref. 26).

TABLE I. Total cross sections (in units of $cm^2$) for electron capture from the $K$ shell of a Li atom by an alpha particle ($^4He^{2+}$) as a function of laboratory impact energy $E$ (keV). The quantization axis for both initial and final bound states is chosen along the incident velocity vector **v**. (a), (b), and (c) relate to Eqs. (4.3a), (4.3b), and (4.3c), respectively. (d) corresponds to the sequence in Eqs. (4.6a)—(4.6d). $X[-N]$ implies $X\times10^{-N}$.

(a)

| | | | $E$ (keV) | | | | | |
|---|---|---|---|---|---|---|---|---|
| $n^f$ | $l^f$ | $m^f$ | 250 | 500 | 700 | 1000 | 1500 | 2500 |
| 1 | 0 | 0 | 2.02 [−16] | 6.57 [−17] | 3.39 [−17] | 1.52 [−17] | 5.22 [−18] | 1.06 [−18] |
| 2 | 0 | 0 | 1.59 [−17] | 7.64 [−18] | 4.35 [−18] | 2.08 [−18] | 7.49 [−19] | 1.55 [−19] |
| 2 | 1 | 0 | 1.38 [−17] | 5.92 [−18] | 3.22 [−18] | 1.38 [−18] | 4.01 [−19] | 5.71 [−20] |
| 2 | 1 | 1 | 1.21 [−18] | 7.86 [−19] | 4.78 [−19] | 2.17 [−19] | 6.41 [−20] | 8.96 [−21] |
| 3 | 0 | 0 | 3.95 [−18] | 2.20 [−18] | 1.29 [−18] | 6.28 [−19] | 2.28 [−19] | 4.73 [−20] |
| 3 | 1 | 0 | 3.54 [−18] | 1.73 [−18] | 1.00 [−18] | 4.53 [−19] | 1.37 [−19] | 2.01 [−20] |
| 3 | 1 | 1 | 2.81 [−19] | 2.10 [−19] | 1.38 [−19] | 6.72 [−20] | 2.10 [−20] | 3.06 [−21] |
| 3 | 2 | 0 | 5.92 [−19] | 2.08 [−19] | 1.05 [−19] | 4.06 [−20] | 9.89 [−21] | 1.02 [−21] |
| 3 | 2 | 1 | 8.98 [−20] | 4.12 [−20] | 2.55 [−20] | 1.13 [−20] | 3.01 [−21] | 3.23 [−22] |
| 3 | 2 | 2 | 6.48 [−21] | 4.12 [−21] | 2.74 [−21] | 1.24 [−21] | 3.23 [−22] | 3.33 [−23] |
| 4 | 0 | 0 | 1.55 [−18] | 9.14 [−19] | 5.44 [−19] | 2.66 [−19] | 9.72 [−20] | 2.02 [−20] |
| 4 | 1 | 0 | 1.41 [−18] | 7.22 [−19] | 4.28 [−19] | 1.97 [−19] | 6.04 [−20] | 8.93 [−21] |
| 4 | 1 | 1 | 1.09 [−19] | 8.49 [−20] | 5.76 [−20] | 2.86 [−20] | 9.12 [−21] | 1.35 [−21] |
| 4 | 2 | 0 | 3.13 [−19] | 1.14 [−19] | 5.90 [−20] | 2.33 [−20] | 5.80 [−21] | 6.08 [−22] |
| 4 | 2 | 1 | 4.70 [−20] | 2.18 [−20] | 1.39 [−20] | 6.38 [−21] | 1.74 [−21] | 1.90 [−22] |
| 4 | 2 | 2 | 3.32 [−21] | 2.12 [−21] | 1.46 [−21] | 6.86 [−22] | 1.84 [−22] | 1.95 [−23] |
| 4 | 3 | 0 | 1.13 [−20] | 3.71 [−21] | 1.78 [−21] | 6.39 [−22] | 1.34 [−22] | 1.03 [−23] |
| 4 | 3 | 1 | 2.98 [−21] | 1.05 [−21] | 6.10 [−22] | 2.55 [−22] | 5.87 [−23] | 4.75 [−24] |
| 4 | 3 | 2 | 4.34 [−22] | 1.92 [−22] | 1.26 [−22] | 5.49 [−23] | 1.27 [−23] | 9.97 [−25] |
| 4 | 3 | 3 | 2.79 [−23] | 1.53 [−23] | 1.05 [−23] | 4.60 [−24] | 1.04 [−24] | 7.93 [−26] |

(b)

| | $E$ (keV) | | | | | |
|---|---|---|---|---|---|---|
| $n^f l^f$ | 250 | 500 | 700 | 1000 | 1500 | 2500 |
| $1s$ | 2.02 [−16] | 6.57 [−17] | 3.39 [−17] | 1.52 [−17] | 5.22 [−18] | 1.06 [−18] |
| $2s$ | 1.59 [−17] | 7.64 [−18] | 4.35 [−18] | 2.08 [−18] | 7.49 [−19] | 1.55 [−19] |
| $2p$ | 1.62 [−17] | 7.50 [−18] | 4.18 [−18] | 1.81 [−18] | 5.29 [−19] | 7.50 [−20] |
| $3s$ | 3.95 [−18] | 2.20 [−18] | 1.29 [−18] | 6.28 [−19] | 2.28 [−19] | 4.73 [−20] |
| $3p$ | 4.10 [−18] | 2.15 [−18] | 1.28 [−18] | 5.87 [−19] | 1.79 [−19] | 2.62 [−20] |
| $3d$ | 7.84 [−19] | 2.99 [−19] | 1.61 [−19] | 6.57 [−20] | 1.66 [−20] | 1.73 [−21] |
| $4s$ | 1.55 [−18] | 9.14 [−19] | 5.44 [−19] | 2.66 [−19] | 9.72 [−20] | 2.02 [−20] |
| $4p$ | 1.63 [−18] | 8.92 [−19] | 5.43 [−19] | 2.54 [−19] | 7.87 [−20] | 1.16 [−20] |
| $4d$ | 4.14 [−19] | 1.62 [−19] | 8.97 [−20] | 3.74 [−20] | 9.64 [−21] | 1.03 [−21] |
| $4f$ | 1.81 [−20] | 6.21 [−21] | 3.28 [−21] | 1.27 [−21] | 2.78 [−22] | 2.19 [−23] |

(c)

| | $E$ (keV) | | | | | |
|---|---|---|---|---|---|---|
| $n$ | 250 | 500 | 700 | 1000 | 1500 | 2500 |
| 1 | 2.02 [−16] | 6.57 [−17] | 3.39 [−17] | 1.52 [−17] | 5.22 [−18] | 1.06 [−18] |
| 2 | 3.20 [−17] | 1.51 [−17] | 8.52 [−18] | 3.89 [−18] | 1.28 [−18] | 2.30 [−19] |
| 3 | 8.83 [−18] | 4.65 [−18] | 2.73 [−18] | 1.28 [−18] | 4.24 [−19] | 7.52 [−20] |
| 4 | 3.62 [−18] | 1.97 [−18] | 1.18 [−18] | 5.59 [−19] | 1.86 [−19] | 3.29 [−20] |

(d)

| | $E$ (keV) | | | | | |
|---|---|---|---|---|---|---|
| Equation | 250 | 500 | 700 | 1000 | 1500 | 2500 |
| (4.6a) | 2.43 [−16] | 7.90 [−17] | 4.08 [−17] | 1.82 [−17] | 6.28 [−18] | 1.28 [−18] |
| (4.6b) | 2.54 [−16] | 9.02 [−17] | 4.77 [−17] | 2.14 [−17] | 7.29 [−18] | 1.43 [−18] |
| (4.6c) | 2.52 [−16] | 9.05 [−17] | 4.81 [−17] | 2.17 [−17] | 7.38 [−18] | 1.45 [−18] |
| (4.6d) | 2.52 [−16] | 9.05 [−17] | 4.82 [−17] | 2.18 [−17] | 7.40 [−18] | 1.45 [−18] |

TABLE II. The same as in Table I, except that this time capture is taking place from the $L$ shell of Li. $X\,[-N]$ implies $X\times10^{-N}$.

(a)

| $n^f$ | $l^f$ | $m^f$ | $E$ (keV) 250 | 500 | 700 | 1000 | 1500 | 2500 |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 3.30 [−18] | 8.39 [−19] | 4.01 [−19] | 1.70 [−19] | 5.56 [−20] | 1.07 [−20] |
| 2 | 0 | 0 | 3.86 [−18] | 3.87 [−19] | 1.08 [−19] | 3.15 [−20] | 8.90 [−21] | 1.62 [−21] |
| 2 | 1 | 0 | 5.24 [−18] | 7.91 [−20] | 4.37 [−20] | 2.18 [−20] | 5.89 [−21] | 6.87 [−22] |
| 2 | 1 | 1 | 3.29 [−19] | 2.30 [−20] | 1.44 [−20] | 5.52 [−21] | 1.23 [−21] | 1.23 [−22] |
| 3 | 0 | 0 | 1.50 [−18] | 1.56 [−19] | 4.04 [−20] | 1.06 [−20] | 2.81 [−21] | 4.99 [−22] |
| 3 | 1 | 0 | 2.95 [−18] | 4.67 [−20] | 1.26 [−20] | 6.76 [−21] | 2.00 [−21] | 2.43 [−22] |
| 3 | 1 | 1 | 1.67 [−19] | 5.44 [−21] | 3.61 [−21] | 1.63 [−21] | 3.99 [−22] | 4.20 [−23] |
| 3 | 2 | 0 | 3.77 [−18] | 7.87 [−21] | 1.52 [−21] | 1.05 [−21] | 2.23 [−22] | 1.59 [−23] |
| 3 | 2 | 1 | 1.18 [−18] | 2.88 [−21] | 1.02 [−21] | 4.65 [−22] | 8.58 [−23] | 5.63 [−24] |
| 3 | 2 | 2 | 9.80 [−20] | 4.25 [−22] | 2.74 [−22] | 8.12 [−23] | 1.18 [−23] | 6.58 [−25] |
| 4 | 0 | 0 | 6.69 [−19] | 7.32 [−20] | 1.86 [−20] | 4.69 [−21] | 1.21 [−21] | 2.13 [−22] |
| 4 | 1 | 0 | 1.42 [−18] | 2.62 [−20] | 5.42 [−21] | 2.88 [−21] | 8.82 [−22] | 1.08 [−22] |
| 4 | 1 | 1 | 8.20 [−20] | 2.30 [−21] | 1.43 [−21] | 6.82 [−22] | 1.73 [−22] | 1.85 [−23] |
| 4 | 2 | 0 | 2.45 [−18] | 7.27 [−21] | 6.92 [−22] | 5.71 [−22] | 1.30 [−22] | 9.49 [−24] |
| 4 | 2 | 1 | 7.12 [−19] | 2.24 [−21] | 4.87 [−22] | 2.50 [−22] | 4.91 [−23] | 3.31 [−24] |
| 4 | 2 | 2 | 5.73 [−20] | 2.09 [−22] | 1.35 [−22] | 4.39 [−23] | 6.68 [−24] | 3.85 [−25] |
| 4 | 3 | 0 | 9.82 [−19] | 2.06 [−21] | 8.78 [−23] | 3.27 [−23] | 4.93 [−24] | 2.15 [−25] |
| 4 | 3 | 1 | 4.36 [−19] | 7.24 [−22] | 4.10 [−23] | 1.80 [−23] | 2.58 [−24] | 1.08 [−25] |
| 4 | 3 | 2 | 7.49 [−20] | 4.54 [−23] | 1.89 [−23] | 6.06 [−24] | 6.93 [−25] | 2.53 [−26] |
| 4 | 3 | 3 | 4.16 [−21] | 6.72 [−24] | 3.52 [−24] | 7.30 [−25] | 6.87 [−26] | 2.23 [−27] |

(b)

| $n^f l^f$ | $E$ (keV) 250 | 500 | 700 | 1000 | 1500 | 2500 |
|---|---|---|---|---|---|---|
| $1s$ | 3.30 [−18] | 8.39 [−19] | 4.01 [−19] | 1.70 [−19] | 5.56 [−20] | 1.07 [−20] |
| $2s$ | 3.86 [−18] | 3.87 [−19] | 1.08 [−19] | 3.15 [−20] | 8.90 [−21] | 1.62 [−21] |
| $2p$ | 5.90 [−18] | 1.25 [−19] | 7.25 [−20] | 3.28 [−20] | 8.35 [−21] | 9.33 [−22] |
| $3s$ | 1.50 [−18] | 1.56 [−19] | 4.04 [−20] | 1.06 [−20] | 2.81 [−21] | 4.99 [−22] |
| $3p$ | 3.29 [−18] | 5.76 [−20] | 1.98 [−20] | 1.00 [−20] | 2.80 [−21] | 3.27 [−22] |
| $3d$ | 6.34 [−18] | 1.45 [−20] | 4.10 [−21] | 2.14 [−21] | 4.19 [−22] | 2.85 [−23] |
| $4s$ | 6.69 [−19] | 7.32 [−20] | 1.86 [−20] | 4.69 [−21] | 1.21 [−21] | 2.13 [−22] |
| $4p$ | 1.58 [−18] | 3.08 [−20] | 8.28 [−21] | 4.25 [−21] | 1.23 [−21] | 1.45 [−22] |
| $4d$ | 3.99 [−18] | 1.22 [−20] | 1.94 [−21] | 1.16 [−21] | 2.41 [−22] | 1.69 [−23] |
| $4f$ | 2.01 [−18] | 3.62 [−21] | 2.15 [−22] | 8.23 [−23] | 1.16 [−23] | 4.85 [−25] |

(c)

| $n$ | $E$ (keV) 250 | 500 | 700 | 1000 | 1500 | 2500 |
|---|---|---|---|---|---|---|
| 1 | 3.30 [−18] | 8.39 [−19] | 4.01 [−19] | 1.70 [−19] | 5.56 [−20] | 1.07 [−20] |
| 2 | 9.75 [−18] | 5.17 [−19] | 1.80 [−19] | 6.43 [−20] | 1.72 [−20] | 2.55 [−21] |
| 3 | 1.11 [−17] | 2.29 [−19] | 6.43 [−20] | 2.28 [−20] | 6.03 [−21] | 8.54 [−22] |
| 4 | 2.25 [−18] | 1.20 [−19] | 2.90 [−20] | 1.02 [−20] | 2.69 [−21] | 3.76 [−22] |

(d)

| Equation | $E$ (keV) 250 | 500 | 700 | 1000 | 1500 | 2500 |
|---|---|---|---|---|---|---|
| (4.6a) | 3.96 [−18] | 1.01 [−18] | 4.82 [−19] | 2.04 [−19] | 6.69 [−20] | 1.28 [−20] |
| (4.6b) | 1.91 [−17] | 1.67 [−18] | 6.93 [−19] | 2.74 [−19] | 8.35 [−20] | 1.48 [−20] |
| (4.6c) | 3.62 [−17] | 1.83 [−18] | 7.15 [−19] | 2.81 [−19] | 8.54 [−20] | 1.50 [−20] |
| (4.6d) | 4.53 [−17] | 1.89 [−18] | 7.20 [−19] | 2.83 [−19] | 8.58 [−20] | 1.50 [−20] |

TABLE III. Total capture cross section $\sigma_i^{(1)}(\Sigma_4)$ in cm$^2$ for reaction (4.1) as a function of laboratory incident energy $E$ (keV). Columns labeled $K$ shell and $L$ shell relate, respectively, to $i\equiv n^i=1$ and $i\equiv n^i=2$. Both sets of these results are obtained from Eq. (4.6d). The last column $K+L$ is obtained from Eq. (4.2) and represents the contribution from both $K$ and $L$ shells of Li($^2S$). $X[-N]$ implies $X\times 10^{-N}$.

| | Shell | | |
|---|---|---|---|
| $E$ (keV) | $K$ | $L$ | $K+L$ |
| 250 | 2.52 [−16] | 4.53 [−17] | 2.97 [−16] |
| 500 | 9.05 [−17] | 1.89 [−18] | 9.24 [−17] |
| 700 | 4.82 [−17] | 7.20 [−19] | 4.89 [−17] |
| 1000 | 2.18 [−17] | 2.83 [−19] | 2.20 [−17] |
| 1500 | 7.40 [−18] | 8.58 [−20] | 7.48 [−18] |
| 2500 | 1.45 [−18] | 1.50 [−20] | 1.47 [−18] |

most probable sources for soft-x-rays in the interstellar medium.[33]

## V. CONCLUSIONS

General expressions have been derived for charge-exchange transition amplitude $T^{(1)}_{nlm;n'l'm'}$ in the first Born approximation of Belkić *et al.*[7] with correct boundary conditions in both entrance and exit channels. The final results are given in terms of a one-dimensional real integral and, hence, can be obtained as easily as in the standard Jackson-Schiff[23] approximation.

We have presented the first results for electron capture from multielectron atoms by bare nuclei, employing an independent-particle model with the Roothaan-Hartree-Fock wave functions. Comprehensive illustrative computations for the $He^{2+}$-Li($^2S$) collision system have been carried out at laboratory energies ranging from 250 to 2500 keV. It is observed that the main contribution to the $K$-shell capture comes from the ground state $1s$ of $He^+$ throughout the energy range under consideration. The final-state distribution of $He^+(n^f)$ tends to broaden considerably when capture takes place from an isolated $L$-shell of Li at intermediate energies. At the lower edge, however, i.e., at $E=250$ keV, the level $n^f=3$ of $He^+$ is found to be preferentially populated for the $L$-shell capture. An overall contribution from the $L$-shell is negligible in comparison with capture from the $K$-shell at energies greater than 250 keV. Agreement with experimental data is satisfactory.

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## APPENDIX A

In this appendix we shall calculate the Fourier transform of the type

$$\mathscr{F}^{(\sigma,\Delta)}_{nlm}(\mathbf{Q})=\sum_{s=0}^{\lambda_l}(-n)_s(-\lambda_l)_s\tilde{B}^{(\sigma,\Delta)}_{vlm}(\mathbf{Q})\frac{(-2)^s}{s!}\ , \quad \text{(A1)}$$

with

$$\tilde{f}(\mathbf{q})=(2\pi)^{-3}\int d\mathbf{r}\,e^{i\mathbf{q}\cdot\mathbf{r}}f(\mathbf{r})\ , \quad \text{(A2)}$$

and

$$B^{(\sigma,\Delta)}_{vlm}(\mathbf{R})=R^{\sigma-1}(vR-\mathbf{v}\cdot\mathbf{R})^{-i\xi}B^{(\Delta)}_{vlm}(\mathbf{R})\ , \quad \text{(A3)}$$

where $B^{(\Delta)}_{vlm}(\mathbf{R})$ is the so-called $B$ function of Filter and Steinborn,[17] i.e.,

$$B^{(\Delta)}_{vlm}(\mathbf{R})=\hat{k}_{\nu-1/2}(R\Delta)\mathscr{Y}_{lm}(\mathbf{R})\ , \quad \text{(A4)}$$

$$\hat{k}_\nu(z)=\left[\frac{2}{\pi}\right]^{1/2}z^\nu K_\nu(z)\ , \quad \text{(A5)}$$

(see also Ref. 15). We shall express the $B$ function in terms of a linear combination of unnormalized Slater-type orbitals,[17]

$$B^{(\Delta)}_{vlm}(\mathbf{R})=\sum_{p=0}^{\nu-1}b_p^\nu\Delta^p\chi^{(\Delta)}_{\bar{p}lm}(\mathbf{R})\ , \quad \text{(A6)}$$

where $\bar{p}=p+l+1$, and

$$\chi^{(\Delta)}_{\bar{p}lm}(\mathbf{R})=R^{\bar{p}-1}e^{-\Delta R}Y_{lm}(\hat{\mathbf{R}})\ , \quad \text{(A7)}$$

$$b_p^\nu=\frac{(2\nu-p-2)!}{(\nu-p-1)!}\frac{2^{p+1-\nu}}{p!}\ . \quad \text{(A8)}$$

Hence, we shall have

$$\mathscr{F}^{(\sigma,\Delta)}_{nlm}(\mathbf{Q})=\sum_{s=0}^{\lambda_l}\sum_{p=0}^{\nu-1}(-n)_s(-\lambda_l)_s b_p^\nu\Delta^p\times\tilde{\chi}^{(\Delta)}_{\bar{p}lm}(\mathbf{Q})\frac{(-2)^s}{s!}\ , \quad \text{(A9)}$$

where

$$\chi^{(\sigma,\Delta)}_{\bar{p}lm}(\mathbf{R})=R^{\sigma-1}(vR-\mathbf{v}\cdot\mathbf{R})^{-i\xi}\chi^{(\Delta)}_{\bar{p}lm}(\mathbf{R})\ . \quad \text{(A10)}$$

The general result of the Fourier transform of functions of the type (A10) is obtained in Appendix B, from which it follows that

$$\tilde{\chi}^{(\sigma,\Delta)}_{\bar{p}lm}(\mathbf{Q})=\frac{(2i)^l}{2\pi^2}\sum_{\kappa=0}^{p_\sigma}\sum_{l_1=0}^{l}\mathscr{I}^{\kappa l}_{pl_1}(\sigma)D^{l_1}_{lm}(\mathbf{Q},\mathbf{v})\quad(p_\sigma=p+\sigma)\ , \quad \text{(A11)}$$

where

$$\mathscr{I}_{pl}^{\kappa l_1}(\sigma)=ab\ {}_3F_2\left[-\frac{\kappa_\sigma}{2},\frac{\kappa_\sigma-1}{2},1-i\gamma_1;\kappa+l+1,-p_\sigma-l;\frac{\Delta^2+Q^2}{\Delta^2}\right], \tag{A12}$$

$$D_{lm}^{l_1}(\mathbf{Q},\mathbf{v})=\sum_{m_1=-l_1}^{+l_1}(l_1m_1\mid lm)\mathscr{Y}_{l_1m_1}(\mathbf{Q})\mathscr{Y}_{l_2m_2}(-i\mathbf{v}), \tag{A13}$$

$$a=\Gamma(1-i\xi)(l+1)_{p_\sigma}\frac{(2\Delta)^{p_\sigma}}{(\Delta^2+Q^2)^{p_\sigma+l+1}}, \tag{A14}$$

$$b=\frac{(1-i\xi)_{l_1}(i\xi)_{l_2}}{x^{i\gamma_2}}\frac{(-p_\sigma)_\kappa(i\gamma_2)_\kappa}{(l+1)_\kappa}\frac{(1-y/x)^\kappa}{\kappa!}, \tag{A15}$$

$$x=\frac{2}{\Delta^2+Q^2}(v\Delta-i\mathbf{Q}\cdot\mathbf{v}),\quad y=v/\Delta, \tag{A16}$$

$$(l_1m_1\mid lm)=\left[4\pi\frac{2l+1}{(2l_1+1)(2l_2+1)}\frac{(l+m)!}{(l_1+m_1)!(l_2+m_2)!}\frac{(l-m)!}{(l_1-m_1)!(l_2-m_2)!}\right]^{1/2}\quad(-l_2\le m_2\le+l_2). \tag{A17}$$

Finally, we shall demonstrate how the double series in Eq. (A9) can be analytically reduced to a single summation. To this end, the summation over $s$ will be exactly carried out. A direct interchange of order of summations over $s$ and $p$ in Eq. (A9) is, however, impossible due to the dependency of upper limit $p_{\max}$ upon $s$ ($p_{\max}\equiv\nu-1=n_r-s$). This difficulty nevertheless can be alleviated by introducing the Heaviside step function $h(n_r-s-p)$ as follows:

$$\begin{aligned}\mathscr{F}_{nlm}^{(\sigma,\Delta)}(\mathbf{Q})&=\sum_{s=0}^{\lambda_l}\sum_{p=0}^{n_r-s}C_{sp}\Delta^p\widetilde{\chi}_{\bar{p}lm}^{(\sigma,\Delta)}(\mathbf{Q})\\&=\sum_{s=0}^{\lambda_l}\sum_{p=0}^{n_r}C_{sp}\Delta^p\widetilde{\chi}_{\bar{p}lm}^{(\sigma,\Delta)}(\mathbf{Q})h(n_r-s-p)\\&=\sum_{p=0}^{n_r}\sum_{s=0}^{\lambda_l}C_{sp}\Delta^p\widetilde{\chi}_{\bar{p}lm}^{(\sigma,\Delta)}(\mathbf{Q})h(n_r-s-p)\\&=\sum_{p=0}^{n_r}\sum_{s=0}^{\min(\lambda_l,n_r-p)}C_{sp}\Delta^p\widetilde{\chi}_{\bar{p}lm}^{(\sigma,\Delta)}(\mathbf{Q}),\end{aligned} \tag{A18}$$

where

$$C_{sp}=(-n)_s(-\lambda_l)_s\frac{(-2)^s}{s!}\frac{(2\nu-p-2)!}{p!(\nu-p-1)!}2^{p-\nu+1}, \tag{A19}$$

$$h(n_r-s-p)=\begin{cases}1, & n_r-s-p\ge0\\0, & n_r-s-p<0.\end{cases} \tag{A20}$$

Fourier transform $\widetilde{\chi}_{\bar{p}lm}^{(\sigma,\Delta)}(\mathbf{Q})$ is independent of dummy index $s$ and, further, the $s$ dependency of coefficient $C_{sp}$ can be factored out by means of the following Pochhammer identities:[34]

$$\begin{aligned}(a)_{n-s}&=(-1)^s\frac{(a)_n}{(1-a-n)_s},\\2^{-2k}(a)_{2k}&=(a/2)_k\left[\frac{a+1}{2}\right]_k,\\(n-2k)!&=\frac{n!}{(-n)_{2k}}.\end{aligned} \tag{A21}$$

Thus we obtain

$$C_{sp}=\left[\frac{(-n)_s(-\lambda_l)_s(-n_r+p)_s}{\left[-n_r+\frac{p}{2}\right]_s\left[-n_r+\frac{p+1}{2}\right]_s}\frac{1}{s!}\right]\times\left[\frac{(2n_r)!}{n_r!}\frac{(-n_r)_p}{(-2n_r)_p}\frac{2^{p-n_r}}{p!}\right]. \tag{A22}$$

Inserting Eq. (A22) into (A18) and carrying out the summation over $s$ we arrive at

$$\mathscr{F}_{nlm}^{(\sigma,\Delta)}(\mathbf{Q})=\frac{(2n_r)!}{n_r!}\sum_{p=0}^{n_r}\frac{(-n_r)_p}{(-2n_r)_p}\ {}_3F_2\left[-n,-\lambda_l,-n_r+p;-n_r+\frac{p}{2},-n_r+\frac{p+1}{2};1\right]\widetilde{\chi}_{\bar{p}lm}^{(\sigma,\Delta)}(\mathbf{Q})\frac{\Delta^p2^{p-n_r}}{p!}, \tag{A23}$$

where ${}_3F_2(-n,-\lambda_l,-n_r+p;-n_r+p/2,-n_r+(p+1)/2;1)$ is the Claussen hypergeometric polynomial of order $\min(\lambda_l,n_r-p)$ with unit argument[19]

$$ {}_3F_2\left[-n,-\lambda_l,-n_r+p;-n_r+\frac{p}{2},-n_r+\frac{p+1}{2};1\right]=\sum_{s=0}^{\min(\lambda_l,n_r-p)}\frac{(-n)_s(-\lambda_l)_s(-n_r+p)_s}{\left[-n_r+\frac{p}{2}\right]_s\left[-n_r+\frac{p+1}{2}\right]_s s!} . \tag{A24}$$

## APPENDIX B

Consider integral $J$ given by

$$ J=(2\pi)^{-3}\int d\mathbf{R}\, e^{i\mathbf{Q}\cdot\mathbf{R}}R^{\sigma-1}(vR-\mathbf{v}\cdot\mathbf{R})^{-i\xi}\chi^{(\Delta)}_{\bar{p}lm}(\mathbf{R}) , \tag{B1}$$

where $\chi^{(\Delta)}_{\bar{p}lm}(\mathbf{R})$ is an unnormalized Slater-type orbital, i.e.,

$$ \chi^{(\Delta)}_{\bar{p}lm}(\mathbf{R})=R^{\bar{p}-1}e^{-\Delta R}Y_{lm}(\hat{\mathbf{R}}) , $$

$$ \bar{p}=p+l+1 \quad (p=0,1,2,\ldots) . \tag{B2}$$

We shall choose the following integral representation for the Coulomb phase factor $(vR-\mathbf{v}\cdot\mathbf{R})^{-i\xi}$ according to Gradshteyn and Ryzhik[18] [Eq. (8.310)]:

$$ (vR-\mathbf{v}\cdot\mathbf{R})^{-i\xi} $$

$$ =\frac{1}{\Gamma(i\xi)}\int_0^\infty dz\, z^{i\xi-1}\exp[-(vR-\mathbf{v}\cdot\mathbf{R})z] , \tag{B3}$$

where an infinitesimally small negative imaginary part $-i\epsilon$ is assumed to be added to parameter $\xi$ in order to assure the convergence of the integral at its upper limit. Upon carrying out the calculation, the limit $\epsilon\to 0^+$ should be taken.

Hence,

$$ J=\frac{1}{\Gamma(i\xi)}\int_0^\infty dz\, z^{i\xi-1}\tilde{\chi}^{(\Delta)}_{\bar{p}lm}(\sigma;\omega,\tau) , \tag{B4}$$

where

$$ \tilde{\chi}^{(\Delta)}_{\bar{p}lm}(\sigma;\omega,\tau)=(2\pi)^{-3}\int d\mathbf{R}\, e^{i\tau\cdot\mathbf{R}-\omega R}R^{\sigma-1}\chi^{(\Delta)}_{\bar{p}lm}(\mathbf{R}) , \tag{B5}$$

$$ \tau=\mathbf{Q}-i\mathbf{v}z, \quad \omega=vz . \tag{B6}$$

Integral (B5) has been calculated by Belkić,[22] with the result

$$ \tilde{\chi}^{(\Delta)}_{\bar{p}lm}(\sigma;\omega,\tau)=(2\pi)^{-3}i^l F^{(\Delta)}_{\bar{p}l}(\sigma;\omega,\tau)\mathscr{Y}_{lm}(\tau) , \tag{B7}$$

where $\mathscr{Y}_{lm}(\tau)=\tau^l Y_{lm}(\hat{\tau})$, and

$$ F^{(\Delta)}_{\bar{p}l}(\sigma;\omega,\tau)=N^\sigma_{pl}\tau_+^{-1-l-p_\sigma/2}C^{l+1}_{p+\nu}(\omega_+/\tau_+^{1/2}) , \tag{B8}$$

$$ N^\sigma_{pl}=4\pi(2l)!!(p+\sigma)!, \quad (2l)!!=2^l l! , $$

$$ \omega_+=\omega+\Delta, \quad \tau_+=\tau^2+\omega_+^2, \quad p_\sigma=p+\sigma , \tag{B9}$$

with $C^\lambda_n(z)$ being the Gegenbauer polynomial [Ref. 18, Eq. (8.930)]. Using the power series representation of $C^\lambda_n(z)$ we can write [Abramowitz and Stegun,[27] (22.3.4)]

$$ F^{(\Delta)}_{\bar{p}l}(\sigma;\omega,\tau)=N^\sigma_{pl}\sum_{p_1=0}^{\left[\frac{p_\sigma}{2}\right]}b^{pl}_{p_1\sigma}\omega_+^{k'}/\tau_+^k , \tag{B10}$$

where $[p_\sigma/2]$ is the largest integer contained in the fraction $p_\sigma/2$, and

$$ b^{pl}_{p_1\sigma}=(-1)^{p_1}2^{k'}(k-1)!/(p_1!k'!l!) , \tag{B11}$$

$$ p_1+p_2=\bar{p}, \quad p_1'+p_2'=p, \quad p_1'=2p_1 , $$

$$ k=p_2+\sigma, \quad k'=p_2'+\sigma . \tag{B12}$$

Quantities $\omega_+$ and $\tau_+$ bear a simple dependence upon integration variable $z$ such as

$$ \tau_+=a_+(1+xz), \quad \omega_+=(1+yz)\Delta , \tag{B13}$$

where

$$ x=\frac{2}{a_+}(v\Delta-i\mathbf{Q}\cdot\mathbf{v}), \quad y=v/\Delta, \quad a_+=Q^2+\Delta^2 . \tag{B14}$$

Furthermore, an addition theorem for the regular solid harmonics $\mathscr{Y}_{lm}(\mathbf{r}_1+\mathbf{r}_2)$ can be applied in order to factor out the $z$ dependence (Seaton,[35] Belkić[36]),

$$ \mathscr{Y}_{lm}(\mathbf{Q})=\sum_{l_1=0}^{l}D^{l_1}_{lm}(\mathbf{Q},\mathbf{v})z^{l_2} , \tag{B15}$$

where

$$ D^{l_1}_{lm}(\mathbf{Q},\mathbf{v})=\sum_{m_1=-l_1}^{+l_1}(l_1m_1\,|\,lm)\mathscr{Y}_{l_1m_1}(\mathbf{Q})\mathscr{Y}_{l_2m_2}(-i\mathbf{v}) , \tag{B16}$$

$$ (l_1m_1\,|\,lm)=\left[4\pi\frac{2l+1}{(2l_1+1)(2l_2+1)}\frac{(l+m)!}{(l_1+m_1)!(l_2+m_2)!}\frac{(l-m)!}{(l_1-m_1)!(l_2-m_2)!}\right]^{1/2} , \tag{B17}$$

$$ l_1+l_2=l, \quad m_1+m_2=m , \quad -l_2\le m_2\le+l_2 . \tag{B18}$$

Thus,

$$ J=\frac{i^l}{(2\pi)^3}\sum_{p_1=0}^{[p_\sigma/2]}\sum_{l_1=0}^{l}N^{pl}_{p_1\sigma}a'D^{l_1}_{lm}(\mathbf{Q},\mathbf{v})\left[\frac{1}{\Gamma(i\xi)}\int_0^\infty dz\, z^{i\xi+l_2-1}(1+xz)^{-k}(1+yz)^{k'}\right] , \tag{B19}$$

where $N_{p_1\sigma}^{pl}=N_{\bar{p}l}^{\sigma}b_{p_1\sigma}^{pl}$ and $a'=\Delta^{k'}/a_+^k$. The integral in the curly brackets is a special case of the Appell hypergeometric function $F_1$ of two variables (Appell and Kampé de Fériet[37]),

$$F_1(a;b,b';c;x,y)=\frac{1}{B(a,c-a)}\int_0^1 dz\, z^{a-1}(1-z)^{c-a-1}\times(1-xz)^{-b}(1-yz)^{-b'}\,, \tag{B20}$$

where $B(x,y)=\Gamma(x)\Gamma(y)/\Gamma(x+y)$. Changing the integration variable $z$ in (B20) according to $z\to z/(1-z)$, we obtain

$$F_1(a;b,b';c;1-x,1-y)=\frac{1}{B(a,c-a)}\int_0^\infty dz\, z^{a-1}(1+z)^{b+b'-c}(1+xz)^{-b}\times(1+yz)^{-b'}\,. \tag{B21}$$

Therefore,

$$K\equiv\frac{1}{\Gamma(i\xi)}\int_0^\infty dz\, z^{i\xi+l_2-1}(1+xz)^{-k}(1+yz)^{k}=\Gamma(1-i\xi)\frac{(i\xi)_{l_2}(1-i\xi)_{\zeta_1-1}}{(\zeta-1)!}\times F_1(l_2+i\xi,k,-k';\zeta;1-x,1-y)\,, \tag{B22}$$

where $(a)_n=\Gamma(a+n)/\Gamma(a)$, $\zeta_1=p_1+l_1+1$ and $\zeta=p_1+l+1$. Next, we shall use the two following properties of the Appell function[37] $F_1$:

$$F_1(a;b,b';c;x,y)=(1-x)^{-a}F_1\left[a;c-b-b',b';c;\frac{x}{x-1},\frac{x-y}{x-1}\right], \tag{B23}$$

$$F_1(a;0,b';c;x,y)={}_2F_1(a,b';c;y)\,, \tag{B24}$$

where ${}_2F_1$ is an ordinary Gauss hypergeometric function of one variable [Gradshteyn and Ryzhik,[18] Eq. (9.100)]. In the present case ${}_2F_1$ is further reduced to a polynomial, since

$$K=\Gamma(1-i\xi)\frac{(i\xi)_{l_2}(1-i\xi)_{\zeta_1-1}}{(\zeta-1)!}x^{-l_2-i\xi}\times{}_2F_1(-k';l_2+i\xi;\zeta;1-y/x)\,. \tag{B25}$$

Finally,

$$J=\frac{(2i)^l}{2\pi^2}\sum_{p_1=0}^{[p_\sigma/2]}\sum_{l_1=0}^{l}\mathscr{G}_{pl}^{p_1l_1}(\sigma)D_{lm}^{l_1}(\mathbf{Q},\mathbf{v})\,, \tag{B26}$$

where

$$\mathscr{G}_{pl}^{p_1l_1}(\sigma)=AB\,{}_2F_1(-k',l_2+i\xi;\zeta;1-y/x)\,, \tag{B27}$$

$$A=(-1)^{p_1}2^{k'}\Gamma(1-i\xi)\times\frac{p_\sigma!(k-1)!(i\xi)_{l_2}(1-i\xi)_{\zeta_1-1}}{p_1!k'!(\zeta-1)!}\,, \tag{B28}$$

$$B=\Delta^{k'}(Q^2+\Delta^2)^{-k}x^{-l_2-i\xi}\,. \tag{B29}$$

If we choose $\mathbf{v}$ as the vector of the quantization axis for Slater-type orbitals, it is at once seen that[36]

$$D_{lm}^{l_1}(\mathbf{Q},\mathbf{v})=(-iv)^{l_2}(l_1\,|\,lm)\mathscr{Y}_{l_1m}(\mathbf{Q})\equiv\hat{D}_{lm}^{l_1}(\mathbf{Q}\cdot\mathbf{v})\,, \tag{B30}$$

where

$$(l_1\,|\,lm)=\left[\frac{2l+1}{2l_1+1}\frac{(l+m)!}{(l_1+m)!l_2!}\frac{(l-m)!}{(l_1-m)!l_2!}\right]^{1/2}, \tag{B31}$$

and Eq. (B26) is subsequently reduced to

$$J=\frac{(2i)^l}{2\pi^2}\sum_{p_1=0}^{[p_\sigma/2]}\sum_{l_1=|m|}^{l}\mathscr{G}_{pl}^{p_1l_1}(\sigma)\hat{D}_{lm}^{l_1}(\mathbf{Q}\cdot\mathbf{v})\,. \tag{B32}$$

Another form of integral $J$ which is an alternative to Eq. (B32) can be obtained by means of the following Pochhammer identities:[34]

$$\begin{aligned}&(a)_k=\Gamma(a+k)/\Gamma(a)\,,\\&(a)_{2k}=2^{2k}\left[\frac{a}{2}\right]_k\left[\frac{a+1}{2}\right]_k,\\&(a)_{n-k}=(-1)^k n!/(a-1-n)_k\,,\\&(n-2k)!=n!/(-n)_{2k}\,,\\&(a+m)_k=(a+k)_m(a)_k/(a)_m\,,\\&(a)_{n+k}=(a)_k(a+k)_n\,.\end{aligned} \tag{B33}$$

The final result is then given by

$$J=\frac{(2i)^l}{2\pi^2}\sum_{\kappa=0}^{p_\sigma}\sum_{l_1=|m|}^{l}\mathscr{I}_{pl}^{\kappa l_1}(\sigma)\hat{D}_{lm}^{l_1}(\mathbf{Q}\cdot\mathbf{v})\,, \tag{B34}$$

where

$$\mathscr{I}_{pl}^{\kappa l_1}(\sigma)=ab\,{}_3F_2\left[-\frac{\kappa_\sigma}{2},-\frac{\kappa_\sigma-1}{2},1-i\gamma_1;\kappa+l+1,-p_\sigma-l;\frac{\Delta^2+Q^2}{\Delta^2}\right], \tag{B35}$$

$$a=\Gamma(1-i\xi)(l+1)_{p_\sigma}\frac{(2\Delta)^{p_\sigma}}{(\Delta^2+Q^2)^{p_\sigma+l+1}}\,, \tag{B36}$$

$$b=\frac{(1-i\xi)_{l_1}(i\xi)_{l_2}}{x^{i\gamma_2}}\frac{(-p_\sigma)_\kappa(i\gamma_2)_\kappa}{(l+1)_\kappa}\frac{(1-y/x)^\kappa}{\kappa!}\ , \tag{B37}$$

$$\kappa_\sigma=p_\sigma-\kappa,\ \ p_\sigma=p+\sigma,\ \ \gamma_1=\xi+il_1,\ \ \gamma_2=\xi-il_2\ . \tag{B38}$$

Here, ${}_3F_2$ is the Claussen generalized hypergeometric polynomial[19]

$${}_3F_2\left[-\frac{\kappa_\sigma}{2},-\frac{\kappa_\sigma-1}{2},1-i\gamma_1;\kappa+l+1,-p_\sigma-l;\frac{\Delta^2+Q^2}{\Delta^2}\right]=\sum_{u=0}^{\left[\frac{\kappa_\sigma}{2}\right]}\frac{(-\kappa_\sigma/2)_u(-\kappa_\sigma/2+\frac{1}{2})_u(1-i\gamma_1)_u}{(\kappa+l+1)_u(-p_\sigma-l)_u u!}\left[\frac{\Delta^2+Q^2}{\Delta^2}\right]^u\ , \tag{B39}$$

where $[\kappa_\sigma/2]$ is the largest integer contained in the fraction $\kappa_\sigma/2$.

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