

Non-partial-wave Coulomb-Born theory for the excitation of many-electron atomic ions II: Numerical description and application

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Abstract. A non-partial-wave Coulomb-Born theory is recently formulated to treat the excitation of many-electron atomic ions for impact by an arbitrary charged particle [Y.B. Duan *et al.*, Phys. Rev. A **56**, 2431 (1997)]. The multiple expansion of the transition matrix element is decomposed into the target form factor and the projectile form factor. These are the matrix elements of the tensor operators between quantum states so that any complicated wave function for the target ion can be employed. In this formal theory, an infinitesimally small positive quantity ε is introduced artificially to guarantee the convergence of integrals. As a supplementary part of the theory, we discuss how to choose the value of ε . It is found that the ε should be taken as functions of the momentum transfer $|\mathbf{q}| = |\mathbf{k}_i - \mathbf{k}_f|$ and multipolarity λ . Illustrations are carried out by calculating the cross-sections for some typical transitions $n_a l_a - n_b l_b$ of hydrogen-like ions for impact by electron, positron, and proton, respectively. The resulting cross-sections are in good agreement with ones produced by using a method available for ion targets with Slater-type orbitals [N.C. Deb, N.C. Sil, Phys. Rev. A **28**, 2806 (1993)]. Comparisons demonstrate that the Coulomb-Born theory with non-partial wave analysis provides a powerful method to treat the excitation of many-electron atomic ions impact by an arbitrary charged particle.

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1 Introduction

The Coulomb-Born (CB) approximation has been used widely to treat atomic ion scattering processes and has been proved to be a useful and reasonable predictor of the processes [1,2]. In the CB approximation, the long-range Coulomb field of the ion is taken care of properly, *i.e.*, the Coulomb wave functions replace the plane wave ones in plane wave Born approximation. Unfortunately, due to the difficulties encountered in mathematics, the applications of the CB approximation for a complex ion system have to depend on partial wave analysis of the projectile or simple analytic wave functions of the target ion [1–6]. However, partial wave treatments require a large number of partial waves at high energy and are not useful for impact by heavy particles. On the other hand, most accurate numerical wave functions can not be used to calculate the process if non-partial wave analysis is employed.

Recently Duan *et al.* [3] noted that if the Coulomb potential is expressed in terms of the spherical harmonic expansion with a parameter integral form it is possible to construct a formal procedure of non-partial wave analysis within the framework of the CB approximation. A formalism in non-partial-wave version has been presented to treat the excitation of many-electron atomic ions for impact by an arbitrary charged particle. In this model, the multiple expansion of the transition matrix element is decomposed into the target form factor and the projectile form factor. These are the matrix elements of the tensor operators between quantum states so that any complicated wave function for the target ion can be employed for the process calculations while the contribution from all partial waves of the projectile is included. This makes it possible to apply the CB approximation to treat the excitation of many-electron atomic ions for impact by a heavy particle.

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In our formal CB non-partial-wave theory, an infinitesimally small positive quantity ε has to be introduced artificially to guarantee the convergence of integrals. As an important part of the theory, it is necessary to investigate how to choose the value of ε because this is very important for subsequent applications of the CB theory. It is found that the ε should be taken as functions of the momentum transfer $|\mathbf{q}| = |\mathbf{k}_i - \mathbf{k}_f|$ and multipolarity λ . Illustrations are carried out by calculating the cross-sections for some typical transitions $n_a l_a - n_b l_b$ of hydrogen-like ions for impact by electron, positron, and proton, respectively. The resulting cross-sections are in good agreement with ones produced by using a method available only for ions with Slater-type analytic wave functions [4]. These data on ε may serve as a guide for subsequent applications of the CB theory to many-electron atomic ions where such a comparison may be not available if an accurate numerically wave function is wanted. Another aim of the present work is to provide systematically high-precision data on excitation cross-section of ions for impact by charged particles, especially by heavy particles. The cross-sections for collision energies from threshold to the high-energy asymptotic limit are required to generate the rate coefficients necessary for many applications in fusion plasma physics and astrophysics. Due to difficulties of obtaining the cross-sections in experiment the calculated data is of great interest [1]. The work on how to combine the wave function code with our dynamics is in progress. In the following papers, we will generalize our CB method to treat many-electron ion targets.

A brief report of the non-partial-wave CB theory has been given recently [3]. To avoid needless repetition, only the useful results for our discussion are cited in the paper. The further description of the approach is presented to supplement the theory.

2 Theory and method

In the CB approximation, the transition matrix for the excitation of an atomic ion of nuclear Z with N electrons is given by

$$T_{ab} = \left\langle F_{\mathbf{k}_f}^{(-)}(Z_f, \mathbf{r}_0) \Phi_b(\mathbf{X}) \left| \sum_j \frac{1}{r_{0j}} \Phi_a(\mathbf{X}) F_{\mathbf{k}_i}^{(+)}(Z_i, \mathbf{r}_0) \right. \right\rangle, \quad (1)$$

where \mathbf{X} represents the set of coordinates of N bound electrons $\{\mathbf{r}_j\}$ and \mathbf{r}_0 does that of the incident electron. The $\Phi_a(\mathbf{X})$ and $\Phi_b(\mathbf{X})$ are the initial and final bound state wave-functions of an ion, $F_{\mathbf{k}_i}^{(+)}(Z_i, \mathbf{r}_0)$ and $F_{\mathbf{k}_f}^{(-)}(Z_f, \mathbf{r}_0)$ are the Coulomb wave functions with outgoing and ingoing boundary conditions in the field of nucleus of charge Z_i and Z_f .

The Coulomb potential in equation (1) can be expressed by the spherical harmonic expansion formula

$$\frac{1}{r_{0j}} = \sum_{\lambda\mu} J_\lambda(r_0, r_j) Y_{\lambda\mu}(\hat{\mathbf{r}}_0) Y_{\lambda\mu}^*(\hat{\mathbf{r}}_j) \quad (2)$$

with

$$J_\lambda(r_0, r_j) = 8 \int dQ j_\lambda(Qr_0) j_\lambda(Qr_j), \quad (3)$$

where $j_\lambda(x)$ is the spherical Bessel function and $Y_{\lambda\mu}(\hat{\mathbf{r}})$ is the spherical harmonic function. The integral of equation (3) is a discontinuous one of Weber and Schafheitlin [7]. The integral over Q is easily performed and leads to the famous Laplace formula

$$\frac{1}{r_{0j}} = \sum_{\lambda\mu} \frac{4\pi}{2\lambda+1} \frac{r_{<}^\lambda}{r_{>}^{\lambda+1}} Y_{\lambda\mu}(\hat{\mathbf{r}}_0) Y_{\lambda\mu}^*(\hat{\mathbf{r}}_j), \quad (4)$$

where $r_{>}$ and $r_{<}$ are the larger and the smaller of r_0 and r_j , respectively. In the conventional CB theory, equation (4) is usually used to expand the Coulomb potential. This leads to that a partial-wave analysis has to be employed to treat the excitation process if any complicated wave function of many-electron ion targets is wanted. Thus, we prefer employing the parameter integral as that in equation (3). Substitution of equation (2) with equation (3) into equation (1) yields

$$T_{ab}(\mathbf{k}_i, \mathbf{k}_f) = (4\pi)^2 \sum_{\lambda\mu} \int_0^\infty dQ D_{\lambda\mu}^{\text{if}}(Q) M_{\lambda\mu}^{ab}(Q), \quad (5)$$

where

$$M_{\lambda\mu}^{ab} = \left\langle \Phi_b(\mathbf{X}) \left| \sum_{j=1}^N j_\lambda(Qr_j) Y_{\lambda\mu}^*(\hat{\mathbf{r}}_j) \right. \Phi_a(\mathbf{X}) \right\rangle \quad (6)$$

and

$$D_{\lambda\mu}^{\text{if}} = \frac{1}{2\pi^2} \left\langle F_{\mathbf{k}_f}^{(-)}(Z_f, \mathbf{r}_0) | j_\lambda(Qr_0) Y_{\lambda\mu}(\hat{\mathbf{r}}_0) | F_{\mathbf{k}_i}^{(+)}(Z_i, \mathbf{r}_0) \right\rangle. \quad (7)$$

It is easily seen that by introducing a mathematical parameter integral the multiple expansion of transition matrix is decomposed into two parts: the target form factor and the projectile distortion one. Equation (6) denotes the so-called form factor that is the matrix element of one-particle tensor operators between the atomic bound states. For discrete excitations, the integral of $Y_{\lambda\mu}(\hat{\mathbf{r}}_j)$ in equation (6) between the bound state wave functions will contribute only for a few values of λ owing to the selection rules for angular momentum eigenstates. Thus, the infinite summation over λ in equation (5) is reduced to a finite one [3].

The projectile distortion factor given by equation (7) is a matrix element of a one-particle tensor of a projectile between an incident wave and a scattered one. By introducing the integral representation of the confluent hypergeometric function and that of the spherical Bessel function, the distortion factor of equation (7) can be rewritten as [3]

$$D_{\lambda\mu}^{\text{if}}(Q) = \frac{Q^{\lambda-1}}{2^{\lambda+1} \pi^2 i (\lambda-1)!} \int_{-1}^1 dt (1-t^2)^{\lambda-1} t S_{\lambda\mu}(\mathbf{k}_i, \mathbf{k}_f, Q, t) \quad (8)$$

with

$$\begin{aligned}
& S_{\lambda\mu}(\mathbf{k}_i, \mathbf{k}_f, Q, t) \\
&= \left\langle F_{\mathbf{k}_f}^{(-)}(Z_f, \mathbf{r}_0) \left| e^{iQr_0t} r_0^{\lambda-1} Y_{\lambda\mu}(\hat{\mathbf{r}}_0) \right| F_{\mathbf{k}_i}^{(+)}(Z_i, \mathbf{r}_0) \right\rangle \\
&= N_{\mathbf{k}_i}^{(+)} N_{\mathbf{k}_f}^{(-)*} \left(-\frac{1}{4\pi^2} \right) \oint_{\Gamma_1} \oint_{\Gamma_2} p(\eta_i, t_1) p(\eta_f, t_2) dt_1 dt_2 \\
&\quad \times \left[\int e^{-\alpha(Q,t)r_0} r_0^{\lambda-1} \exp(i\mathbf{q}' \cdot \mathbf{r}_0) Y_{\lambda\mu}(\hat{\mathbf{r}}_0) d\mathbf{r}_0 \right], \quad (9)
\end{aligned}$$

where

$$\begin{aligned}
N_{\mathbf{k}_i}^{(+)} &= \exp(\pi\eta_i/2) \Gamma(1 - i\eta_i), \\
N_{\mathbf{k}_f}^{(-)} &= \exp(\pi\eta_f/2) \Gamma(1 + i\eta_f), \\
\mathbf{q}' &= \mathbf{k}_i(1 - t_1) - \mathbf{k}_f(1 - t_2),
\end{aligned}$$

and

$$\alpha(Q, t) = \varepsilon - iQt - ik_i t_1 - ik_f t_2, \quad \varepsilon \rightarrow 0^+. \quad (10)$$

It is in equation (9) that an infinitesimally small positive quantity ε is introduced artificially to guarantee the convergence of integral. This is the so-called regularization procedure applied usually in atomic physics to treat divergent integrals.

After carrying out sequentially the integrations over r_0 , t_1 , and t_2 , equation (9) becomes an analytic form [3]

$$S_{\lambda\mu}(\mathbf{k}_i, \mathbf{k}_f, Q, t) = 4\pi N_{\mathbf{k}_i}^{(+)} N_{\mathbf{k}_f}^{(-)*} (2i)^\lambda \lambda! H, \quad (11)$$

where

$$\begin{aligned}
H &= \sum_{l'=0}^{\lambda} C_{l'}^{l''} \sum_{v=0}^{l''} C_v^{l''} \sum_{h=0}^{l'} \frac{(\alpha)_h (-l')_h (\epsilon_2)_h}{h! (\gamma)_h} \\
&\quad \times {}_2F_1(\alpha + h, \beta; \gamma + h; \epsilon_1) \quad (12)
\end{aligned}$$

with

$$\begin{aligned}
C_{l'}^{l''} &= \frac{2(-1)^{l''} [\pi(2\lambda + 1)(\lambda + \mu)! (\lambda - \mu)!]^{1/2} (1 - i\eta_i)_\lambda (1 - i\eta_f)_{l''}}{[(2l' + 1)(2l'' + 1)(l'!)^2 (l'' + \mu)! (l'' - \mu)!]^{1/2} \lambda! l''!} \\
&\quad \times k_i^{l'} k_f^{l''} Y_{l'0}(\hat{\mathbf{k}}_i) Y_{l''\mu}(\hat{\mathbf{k}}_f),
\end{aligned}$$

$$C_v^{l''} = \frac{(i\eta_i)_v (-l'')_v}{v! (-\lambda + i\eta_i)_v} X^{-O} X_1^{-R} (1 - Y_1/X_1)^{-\alpha},$$

$$l'' = \lambda - l', \quad O = \lambda + 1 - v - i\eta_i, \quad R = v + i\eta_i,$$

$$X = (\varepsilon - iQt)^2 + k_i^2 + k_f^2 - 2\mathbf{k}_i \cdot \mathbf{k}_f,$$

$$Y = 2[i(\varepsilon - iQt)k_f + k_f^2 - \mathbf{k}_i \cdot \mathbf{k}_f],$$

$$X_1 = (\varepsilon - iQt - ik_i)^2 + k_f^2,$$

$$Y_1 = 2k_f[i(\varepsilon - iQt) + k_i + k_f],$$

$$\epsilon_1 = \frac{Y_1/X_1 - Y/X}{Y_1/X_1 - 1}, \quad \epsilon_2 = \frac{Y_1/X_1}{Y_1/X_1 - 1},$$

$$\alpha = i\eta_f, \quad \beta = O, \quad \gamma = l'' + 1,$$

where $(\beta)_\alpha$ is the Pochhammer symbol

$$\begin{aligned}
(\beta)_\alpha &= \beta(\beta + 1)(\beta + 2) \cdots (\beta + \alpha - 1), \quad (\beta)_0 = 1, \\
&\quad (\alpha = 0, 1, 2, \dots),
\end{aligned}$$

and ${}_2F_1(\alpha, \beta; \gamma; z)$ is the Gaussian hypergeometric function.

For $\lambda = 0$, the distortion factor $D_{\lambda\mu}^{\text{if}}(Q)$ is further reduced to an analytic form

$$D_{00}^{\text{if}}(Q) = \frac{Q^{-1}}{4\pi^2 i} [S_{00}(\mathbf{k}_i, \mathbf{k}_f, Q, 1) - S_{00}(\mathbf{k}_i, \mathbf{k}_f, Q, -1)]. \quad (13)$$

At this stage, for an arbitrary many-electron ion system the transition matrix element in equation (1) is reduced to a two-dimensional integral over Q and t (and r_j) which is to be evaluated numerically.

It is noted that the first and third parameters of the hypergeometric function ${}_2F_1(\alpha, \beta; \gamma; z)$ in equation (12) increase gradually by unity up to a certain limit. This fact can be exploited with advantage for the evaluation of the series. If we calculate only two such successive functions, the others can be obtained from these two by repeated use of contiguous relations for the ${}_2F_1(\alpha, \beta; \gamma; z)$ function. This programming scheme saves greatly the computer times for a larger value of the multipolarity λ in equation (5).

3 Determination of ε and numerical results

To investigate how to choose the value of ε , we simply analyze the structure of the formulas given in our theory. It is found from equation (12) that the singularities are encountered at $Qt = \pm q$ in the expressions of X , X_1 , and $Y_1 - X_1$, *i.e.*,

$$X = q^2 \left[1 - \left(\frac{Qt}{q} + i\frac{\varepsilon}{q} \right)^2 \right], \quad (14)$$

$$X_1 = k_f^2 \left[1 - \left(\frac{Qt + k_i}{k_f} + i\frac{\varepsilon}{k_f} \right)^2 \right], \quad (15)$$

$$Y_1 - X_1 = (k_i + k_f)^2 \left(1 + \frac{Qt}{k_i + k_f} + i\frac{\varepsilon}{k_i + k_f} \right)^2, \quad (16)$$

where q is the magnitude of the momentum transfer vector $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$. From equation (10) we know that the ε must be infinitesimally small to guarantee: (a) the convergence of integral and (b) obtaining an interest value of the integral. Equations (14–16) indicate that the ratios ε/q , ε/k_f , and $\varepsilon/(k_i + k_f)$ should be taken as infinitesimally small quantities trending towards zero to guarantee the convergence of integral. Without loss of generality, the ε can be taken as

$$\varepsilon = \delta q. \quad (17)$$

Table 1. Integrated cross-sections $Z^4\sigma$ (10^{-17} cm²) of the $1s-2s$ excitation of hydrogen-like ions for impact by electron and positron, respectively.

| x | e | $Z = 2$ | e | $Z = 8$ | e | $Z = 50$ |
|-----|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|
| 2 | 2.4391 ^a | 2.4391 ^b | 2.5952 ^a | 2.5952 ^b | 2.6365 ^a | 2.6365 ^b |
| 3 | 1.6680 | 1.6680 | 1.7520 | 1.7520 | 1.7726 | 1.7726 |
| 5 | 1.0192 | 1.0192 | 1.0555 | 1.0555 | 1.0644 | 1.0644 |
| 10 | 0.5157 | 0.5157 | 0.5263 | 0.5263 | 0.5291 | 0.5291 |
| 20 | 0.2592 | 0.2592 | 0.2621 | 0.2621 | 0.2629 | 0.2629 |
| 30 | 0.1731 | 0.1731 | 0.1744 | 0.1744 | 0.1748 | 0.1748 |
| 40 | 0.1299 | 0.1299 | 0.1307 | 0.1307 | 0.1309 | 0.1309 |
| x | e^+ | $Z = 2$ | e^+ | $Z = 8$ | e^+ | $Z = 50$ |
| 2 | 0.8775 ^a | 0.8775 ^b | 0.3232 ^a | 0.3232 ^b | 0.2347 ^a | 0.2347 ^b |
| 3 | 1.0610 | 1.0610 | 0.7016 | 0.7016 | 0.6110 | 0.6110 |
| 5 | 0.8361 | 0.8361 | 0.7204 | 0.7204 | 0.6851 | 0.6851 |
| 10 | 0.4762 | 0.4762 | 0.4554 | 0.4554 | 0.4489 | 0.4489 |
| 20 | 0.2500 | 0.2500 | 0.2458 | 0.2458 | 0.2446 | 0.2446 |
| 30 | 0.1691 | 0.1691 | 0.1674 | 0.1674 | 0.1669 | 0.1669 |
| 40 | 0.1277 | 0.1277 | 0.1268 | 0.1268 | 0.1265 | 0.1265 |

^a The results obtained using Deb and Sil's method [4].

^b The ones obtained in the present work.

By trial and error, we found that the δ depends on the multipolarity λ . For practical calculations the δ can be taken as

$$\delta = \begin{cases} 10^{-6}, & \text{for } 1s-2s, \text{ where } \lambda = 0 \\ 10^{-5}, & \text{for } 1s-2p, \text{ where } \lambda = 1. \end{cases} \quad (18)$$

Thus, the ε will depend on the magnitude of momentum transfer vector \mathbf{q} and the multipolarity λ .

Using equations (17, 18), we calculated some typical excitation cross-sections such as $1s-2s$ and $1s-2p$ of the hydrogen-like ions with $Z = 2, 8, 50$ by electron and positron impact at incident energies $x = \Delta E/E = 2 \sim 40$, where E is the collision energy and ΔE is the excitation energy. In order to check our results we also calculated the same excitation processes by using a method only for ions with Slater-type wave functions proposed by Deb and Sil. The comparisons between the two kind of calculated results are shown in Tables 1 and 2, respectively. As shown in Tables 1 and 2, the present results are in excellent agreement with those produced by Deb and Sil's method [4] and have high accuracy at intermediate and high energy regions.

On the other hand, in order to investigate if our conclusions about the ε are still valid for impact by a heavy charged particle, we calculated the cross-sections of $1s-2s$ and $1s-2p$ excitation of He^+ by proton impact at incident energies $x = 10^2 \sim 10^4$ using the two methods. The resulting cross-sections from the two methods, as shown in Table 3, are in good agreement with each other.

Similarly, the values of δ in equation (18) can be determined for higher excitations. It should be emphasized that the definitions of ε and δ in equations (17, 18) are of common significance. These data on ε may serve as a guide for subsequent applications of the CB theory to

Table 2. Integrated cross-sections $Z^4\sigma$ (10^{-16} cm²) of the $1s-2p$ excitation of hydrogen-like ions for impact by electron and positron, respectively.

| x | e | $Z = 2$ | e | $Z = 8$ | e | $Z = 50$ |
|-----|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|
| 2 | 1.3843 ^a | 1.3843 ^b | 1.5019 ^a | 1.5018 ^b | 1.5315 ^a | 1.5315 ^b |
| 3 | 1.2133 | 1.2133 | 1.2636 | 1.2635 | 1.2766 | 1.2766 |
| 5 | 0.9653 | 0.9653 | 0.9800 | 0.9800 | 0.9840 | 0.9840 |
| 10 | 0.6540 | 0.6540 | 0.6556 | 0.6556 | 0.6560 | 0.6560 |
| 20 | 0.4158 | 0.4158 | 0.4155 | 0.4155 | 0.4154 | 0.4154 |
| 30 | 0.3122 | 0.3122 | 0.3120 | 0.3119 | 0.3118 | 0.3118 |
| 40 | 0.2529 | 0.2529 | 0.2526 | 0.2526 | 0.2526 | 0.2526 |
| x | e^+ | $Z = 2$ | e^+ | $Z = 8$ | e^+ | $Z = 50$ |
| 2 | 0.7619 ^a | 0.7619 ^b | 0.4678 ^a | 0.4678 ^b | 0.4003 ^a | 0.4003 ^b |
| 3 | 0.9907 | 0.9907 | 0.8549 | 0.8549 | 0.8142 | 0.8142 |
| 5 | 0.9128 | 0.9128 | 0.8824 | 0.8824 | 0.8726 | 0.8726 |
| 10 | 0.6498 | 0.6498 | 0.6478 | 0.6478 | 0.6471 | 0.6471 |
| 20 | 0.4168 | 0.4168 | 0.4173 | 0.4173 | 0.4174 | 0.4174 |
| 30 | 0.3132 | 0.3132 | 0.3136 | 0.3136 | 0.3137 | 0.3137 |
| 40 | 0.2536 | 0.2536 | 0.2539 | 0.2539 | 0.2540 | 0.2540 |

^{a,b} The same as in Table 1.

Table 3. Integrated cross-sections $Z^4\sigma$ (cm²) of the $1s-2s$, $2p$ excitation of hydrogen-like ion He^+ for impact by proton.

| x | $1s-2s$ | $\times 10^{-17}$ | $1s-2p$ | $\times 10^{-16}$ |
|-----------------|---------------------|---------------------|---------------------|---------------------|
| 1×10^2 | 0.8940 ^a | 0.8940 ^b | 0.0448 ^a | 0.0448 ^b |
| 5×10^2 | 5.0249 | 5.0249 | 0.9925 | 0.9925 |
| 8×10^2 | 4.9788 | 4.9788 | 1.3886 | 1.3886 |
| 1×10^3 | 4.6902 | 4.6902 | 1.5245 | 1.5245 |
| 5×10^3 | 1.6448 | 1.6448 | 1.3172 | 1.3172 |
| 8×10^3 | 1.0872 | 1.0872 | 1.0664 | 1.0663 |
| 1×10^4 | 0.8863 | 0.8863 | 0.9494 | 0.9494 |

^{a,b} The same as in Table 1.

many-electron atomic ions where such a comparison may not be available if an accurate numerically wave function is wanted.

4 Conclusion

From the analysis given in the present work, we found that the cross-sections obtained by using a formal non-partial-wave analysis method are in quite excellent agreement with those produced by Deb and Sil's method [4] and by the partial-wave analysis method [8] in the CB approximation. This means that the presented non-partial-wave CB method can be used to provide useful and reliable cross-sections for the excitation of other complicated ion systems with numerical wave functions by an arbitrary particle impact.

We have shown that the Coulomb-Born theory with non-partial wave analysis provides a powerful method to compute the cross-sections for the excitation of many-electron atomic ions impact by an arbitrary charged

particle. From the viewpoint of methodology, our approach has following distinguishing features:

- (a) for the practical application it should be emphasized that the appearing of the form factor with harmonic function is of great significance because the most accurate multi-configuration Hartree-Fock wave-function can be used for the process calculation;
- (b) all the calculations are reduced to two-dimensional integration at the most;
- (c) the results include the contributions from all partial waves;
- (d) the differential cross-sections can be produced.

A systemic improvement of the CB approach by including important corrections such as the exchange effect, the relativistic effect, the second or higher order terms and so on, in a formal way remains an interesting task for future work. Finally, we expect that our formalism will be able to open up new vistas of the CB approximation.

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