Non-partial-wave Coulomb-Born theory for the excitation of many-electron atomic ions

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A formal theory for the evaluation of the cross section for the excitation of many-electron atomic ion within the framework of the Coulomb-Born approximation is formulated in non-partial-wave version, in which the multiple expansion of the transition matrix element is decomposed into two parts: the target form factor and the projectile distortion 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. Thus it becomes possible to apply Coulomb-Born theory to treat the excitation of many-electron atomic ions for impact by charged particles, especially heavy particles. As an illustration, the $1s$-$2s$ and $1s$-$2p$ excitation cross sections of hydrogenlike ions by electron impact are calculated for a wide range of energies using the Coulomb-Born formal analysis. [S1050-2947(97)00409-5]

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The inelastic scattering process of atomic ions by charged-particle impact is important as one of the basic atomic processes in plasma physics and astrophysics. Theoretical investigations of such problems are of not only practical interest but also more fundamental interest [1]. Over the past half-century, numerous approximation methods have been proposed for the process calculation, among which the plane-wave Born approximation is the simplest one. Although the plane-wave Born approximation is limited to describing collisions of fast incident particles with atoms, it appears to be one with universal acceptance. As is well known, for the plane-wave Born approximation, the projectile wave is denoted by the plane wave $\exp(i\mathbf{k}\cdot\mathbf{r})$, and the projectile-dependent terms can be integrated out using the Bethe integral [2]. This kind of simplification occurs only for the plane-wave Born approximation and has substantial merits in comparison with other approximate ansätze: (a) the evaluations of the transition matrix are only related to the coordinates of target electrons, and the matrix element involved is expanded as summations of one-particle tensor operators; (b) the calculations provide contributions from all partial waves of the projectile; and (c) some formal procedures for the evaluations of the reduced matrix elements using arbitrary complicated wave functions have been developed for public use.

For an atomic ion-scattering system, the long-range Coulomb field of the ion yields a notable effect, and should be taken care of properly. As an improvement over the Born approximation, the Coulomb-Born (CB) approximation has been used widely to treat the atomic scattering process, and has been proved to be a useful and reasonable predictor of the process [1]. In the CB approximation, the Coulomb wave functions replace the plane-wave ones in the 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 a partial-wave analysis of the projectile or simple analytic wave functions of the target ion [3–7]. 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, if non-partial-wave analysis is employed, most accurate numerical wave functions cannot be used to calculate the process so far.

Recently we noted that if the Coulomb potential is expressed in terms of the spherical harmonic expansion with a parameter integral form, it is also possible to construct a formal procedure of non-partial-wave analysis in the CB approximation, in which a technique similar to that applied for the plane-wave Born approximation can be utilized with few modifications. This means that the CB approximation also has the same merits as those mentioned above for the plane-wave Born approximation. Thus our method may open up vistas for the CB approximation.

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

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

where $\mathbf{X}$ represents the set of coordinates of N bound electrons $\{\mathbf{r}_j\}$, and $\mathbf{r}_0$ that of the incident electron. $\Phi_a(\mathbf{X})$ and $\Phi_b(\mathbf{X})$ are the initial and final bound-state wave functions of an ion, and $F_{\mathbf{k}_i}^{(+)}(Z_i,\mathbf{r}_0)$ 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, explicitly:

$$\begin{aligned}F_{\mathbf{k}_i}^{(+)}(Z_i,\mathbf{r}_0)&=N_{\mathbf{k}_i}^{(+)}\exp(i\mathbf{k}_i\cdot\mathbf{r}_0)\,{}_1F_1(i\eta_i,1,ik_ir_0-i\mathbf{k}_i\cdot\mathbf{r}_0),\\ F_{\mathbf{k}_f}^{(-)}(Z_f,\mathbf{r}_0)&\\ &=N_{\mathbf{k}_f}^{(-)}\exp(i\mathbf{k}_f\cdot\mathbf{r}_0)\,{}_1F_1(-i\eta_f,1,-ik_fr_0-i\mathbf{k}_f\cdot\mathbf{r}_0),\end{aligned} \tag{2}$$

with

$$N_{\mathbf{k}_i}^{(+)}=\exp\left(\frac{\pi}{2}\eta_i\right)\Gamma(1-i\eta_i),$$

$$N_{\mathbf{k}_f}^{(-)}=\exp\left(\frac{\pi}{2}\eta_f\right)\Gamma(1+i\eta_f),$$

where $\eta_i=Z_i/k_i$ and $\eta_f=Z_f/k_f$.

Now the Coulomb potential can be expressed by the spherical harmonic expansion formula

$$\frac{1}{r_{0j}}=\sum_{\lambda\mu} J_\lambda(r_0,r_j)Y_{\lambda\mu}(\hat{\mathbf{r}}_0)Y^*_{\lambda\mu}(\hat{\mathbf{r}}_j), \tag{3}$$

with

$$J_\lambda(r_0,r_j)=8\int dQ\; j_\lambda(Qr_0)j_\lambda(Qr_j), \tag{4}$$

where $j_\lambda(x)$ is spherical Bessel function and $Y_{\lambda\mu}(\hat{\mathbf{r}})$ is the spherical harmonic function. The integral of Eq. (4) is the discontinuous one of Weber and Schafheitlin [8]. We prefer employing the parameter integral form in Eq. (4), although the integral over Q is easily performed and leads to an analytic function. Substitution of Eq. (3) with Eq. (4) into Eq. (1) yields

$$T^{CB}_{ab}(\mathbf{k}_i,\mathbf{k}_f)=(4\pi)^2\sum_{\lambda\mu}\int_0^\infty dQ\; D^{if}_{\lambda\mu}(Q)M^{ab}_{\lambda\mu}(Q), \tag{5}$$

where

$$M^{ab}_{\lambda\mu}=\langle\Phi_b(\mathbf{X})|\sum_{j=1}^{N} j_\lambda(Qr_j)Y^*_{\lambda\mu}(\hat{\mathbf{r}}_j)|\Phi_a(\mathbf{X})\rangle \tag{6}$$

and

$$D^{if}_{\lambda\mu}=\frac{1}{2\pi^2}\langle F^{(-)}_{\mathbf{k}_f}(Z_f,\mathbf{r}_0)|j_\lambda(Qr_0)Y_{\lambda\mu}(\hat{\mathbf{r}}_0)|F^{(+)}_{\mathbf{k}_i}(Z_i,\mathbf{r}_0)\rangle. \tag{7}$$

It is easily seen that by introducing a mathematical parameter integral the multiple expansion of the 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 Eq. (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. For example, if the one-particle ones in the multiconfiguration wave functions of an ion system are taken as

$$\phi_a(\mathbf{r}_j)=Y_{l_am_a}(\hat{\mathbf{r}}_j)P_a(r_j)/r_j,$$

$$\phi_b(\mathbf{r}_j)=Y_{l_bm_b}(\hat{\mathbf{r}}_j)P_b(r_j)/r_j. \tag{8}$$

Equation (6) becomes

$$M^{ab}_{\lambda\mu}=\sum_{j=1}^{N} {}^j\Lambda(\lambda\mu)\,{}^jy_\lambda, \tag{9}$$

where

$${}^jy_\lambda=\int P_b(r_j)j_\lambda(Qr_j)P_a(r_j)dr_j \tag{10}$$

and

$${}^j\Lambda(\lambda\mu)=\frac{1}{2\sqrt{\pi}}(-1)^{m_a}\prod(l_al_b\lambda)\begin{pmatrix} l_a & \lambda & l_b\\ 0 & 0 & 0\end{pmatrix}\times\begin{pmatrix} l_a & \lambda & l_b\\ -m_a & \mu & m_b\end{pmatrix} \tag{11}$$

with the selection rules (a) $|l_b-l_a|\leqslant\lambda\leqslant l_b+l_a$, (b) $l_a+l_b+\lambda$ is even, and (c) $\mu=m_a-m_b$. In Eq. (11), $\Pi(j_1j_2\ldots)=(2j_1+1)^{1/2}(2j_2+1)^{1/2}\ldots$, the usual notation for the Wigner $3-j$ coefficient is used.

The projectile distortion factor given by Eq. (7) is a matrix element of a one-particle tensor of a projectile between an incident wave and a scattered one. The key point of the present work is to simplify the distortion factor. By introducing the integral representation of the confluent hypergeometric function [9]

$${}_1F_1(i\eta,1,z)=\frac{1}{2i\pi}\oint_\Gamma p(\eta,t)e^{zt}dt, \tag{12}$$

with

$$p(\eta,t)=t^{i\eta-1}(1-t)^{-i\eta},$$

where Γ indicates a closed contour encircling each of the two points 0 and 1 once counterclockwise, and that of the spherical Bessel function [8]

$$j_\lambda(z)=\frac{z^\lambda}{2^{\lambda+1}\lambda!}\int_{-1}^{1}e^{izx}(1-x^2)^\lambda dx, \tag{13}$$

the distortion factor of Eq. (7) can be rewritten as

$$D^{if}_{\lambda\mu}(Q)=\frac{Q^{\lambda-1}}{2^{\lambda+1}\pi^2 i(\lambda-1)!}\times\int_{-1}^{1}dt(1-t^2)^{\lambda-1}tS_{\lambda\mu}(\mathbf{k}_i,\mathbf{k}_f,Q,t), \tag{14}$$

with

TABLE I. Total cross sections $Z^4\sigma$ (10^{-17} cm^2) for the $1s$-$2s$ excitation of hydrogenlike ions by electron impact.

x	$Z=2$			$Z=8$			$Z=50$		
2	2.439 [a]	2.4397[b]	2.440 [c]	2.595 [a]	2.5954[b]	2.595 [c]	2.636 [a]	2.6365[b]	2.637 [c]
3	1.668	1.6684	1.668	1.752	1.7521	1.752	1.773	1.7726	1.773
4	1.266	1.2660	1.266	1.318	1.3185	1.319	1.331	1.3313	1.332
5	1.019	1.0194	1.019	1.055	1.0555	1.056	1.064	1.0644	1.065
10	0.5157	0.5158	0.5158	0.5263	0.5264	0.5265	0.5291	0.5291	0.5292
15	0.3450	0.3451	0.3451	0.3500	0.3501	0.3501		0.3514	0.3515
20	0.2592	0.2592	0.2592	0.2621	0.2621	0.2621		0.2629	0.2629
25	0.2075	0.2076	0.2076	0.2095	0.2095	0.2095		0.2100	0.2100
30	0.1731	0.1731	0.1731	0.1744	0.1744	0.1744		0.1748	0.1748
40		0.1300	0.1299		0.1307	0.1307		0.1309	0.1309

[a]The results obtained using partial-wave analysis [7].
[b]The ones obtained in the present work.
[c]The ones obtained using analytic resolution [6].

$$S_{\lambda\mu}(\mathbf{k}_i,\mathbf{k}_f,Q,t)$$
$$=\langle F^{(-)}_{\mathbf{k}_f}(Z_f,\mathbf{r}_0)|e^{iQr_0t}r_0^{\lambda-1}Y_{\lambda\mu}(\hat{\mathbf{r}}_0)|F^{(+)}_{\mathbf{k}_i}(Z_i,\mathbf{r}_0)\rangle$$
$$=N^{(+)}_{\mathbf{k}_i}N^{(-)}_{\mathbf{k}_f}{}^{*}\left(-\frac{1}{4\pi^2}\right)$$
$$\times\oint_{\Gamma_1}\oint_{\Gamma_2}p(\eta_i,t_1)p(\eta_f,t_2)dt_1dt_2$$
$$\times\left[\int e^{-\alpha(Q,t)r_0}r_0^{\lambda-1}\exp(i\mathbf{q}\cdot\mathbf{r}_0)Y_{\lambda\mu}(\hat{\mathbf{r}}_0)d\mathbf{r}_0\right], \quad (15)$$

where

$$\alpha(Q,t)=\varepsilon-iQt-ik_it_1-ik_ft_2 \quad (\varepsilon\to 0^+), \quad (16)$$

$$\mathbf{q}=\mathbf{k}_i(1-t_1)-\mathbf{k}_f(1-t_2); \quad (17)$$

here infinitesimally small positive quantity ε is introduced artificially to guarantee the convergence.

For $\lambda=0$, the distortion factor $D^{if}_{\lambda\mu}(Q)$ becomes a analytic form

$$D^{if}_{00}(Q)=\frac{Q^{-1}}{4\pi^2 i}[S_{00}(\mathbf{k}_i,\mathbf{k}_f,Q,1)-S_{00}(\mathbf{k}_i,\mathbf{k}_f,Q,-1)]. \quad (18)$$

For $\lambda\geqslant 1$, using the formula

$$\int e^{-\alpha r}r^{L-1}\exp(i\mathbf{K}\cdot\mathbf{r})Y_{LM}(\hat{\mathbf{r}})d\mathbf{r}$$
$$=4\pi(2i)^L L!\frac{K^L Y_{LM}(\hat{\mathbf{K}})}{(K^2+\alpha^2)^{L+1}}, \quad (19)$$

we obtain

$$S_{\lambda\mu}(\mathbf{k}_i,\mathbf{k}_f,Q,t)=N^{(+)}_{\mathbf{k}_i}N^{(-)}_{\mathbf{k}_f}{}^{*}4\pi(2i)^\lambda\lambda!H, \quad (20)$$

with

$$H=\left(-\frac{1}{4\pi^2}\right)\oint_{\Gamma_1}\oint_{\Gamma_2}\frac{q^\lambda Y_{\lambda\mu}(\hat{\mathbf{q}})}{[\alpha(q,t)^2+q^2]^{\lambda+1}}$$
$$\times p(\eta_i,t_1)p(\eta_f,t_2)dt_1dt_2. \quad (21)$$

After carrying out the integrations over t_1 and t_2 in Eq. (21), H becomes [5]

$$H=\sum_{l'=0}^{\lambda}C^{l''}_{l'}\sum_{v=0}^{l''}C^{l'}_{v}\sum_{h=0}^{l'}\frac{(\alpha)_h(-l')_h(\epsilon_2)^h}{h!(\gamma)_h}$$
$$\times {}_2F_1(\alpha+h,\beta;\gamma+h;\epsilon_1), \quad (22)$$

with

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

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

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

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

TABLE II. Total cross sections $Z^4\sigma$ (10^{-16} cm^2) for the $1s$-$2p$ excitation of hydrogenlike ions by electron impact.

x	$Z=2$			$Z=8$			$Z=50$		
2	1.384 [a]	1.3850[b]	1.385 [c]	1.502 [a]	1.5024[b]	1.502 [c]	1.532 [a]	1.5317[b]	1.532 [c]
3	1.213	1.2134	1.214	1.264	1.2638	1.264	1.277	1.2766	1.277
4	1.074	1.0748	1.075	1.100	1.1004	1.101	1.107	1.1071	1.107
5	0.9652	0.9655	0.9655	0.9800	0.9801	0.9803	0.9839	0.9840	0.9842
10	0.6540	0.6541	0.6541	0.6556	0.6556	0.6557	0.6560	0.6560	0.6562
15	0.5049	0.5050	0.5051	0.5049	0.5050	0.5051		0.5049	0.5051
20	0.4158	0.4159	0.4159	0.4155	0.4155	0.4156		0.4154	0.4155
25	0.3557	0.3559	0.3559	0.3554	0.3554	0.3555		0.3553	0.3554
30	0.3122	0.3123	0.3124	0.3119	0.3119	0.3121		0.3119	0.3120
40		0.2529	0.2529		0.2526	0.2527		0.2525	0.2526

[a–c]The same as in Table I.

$$X_1=(\varepsilon-iQt-ik_i)^2+k_f^2, \quad Y_1=2k_f[i(\varepsilon-iQt)+k_i+k_f],$$

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

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

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

$$(\beta)_\alpha=\beta(\beta+1)(\beta+2)\cdots(\beta+\alpha-1),$$

$$(\beta)_0=1 \quad (\alpha=0,1,2,\ldots),$$

and ${}_2F_1(\alpha,\beta;\gamma;z)$ is the Gaussian hypergeometric function. At this stage, for an arbitrary many-electron ion system, the transition matrix element in Eq. (1) is reduced to two-dimensional integral over Q and t (and r_j), which is to be evaluated numerically.

For a consistency check on our method, we calculated the $1s$-$2s$ and $1s$-$2p$ excitation cross sections of hydrogenlike ions with $Z=2$, 8, and 50 by electron impact at energies $x=2-40$ in threshold units, and compared them with those obtained by partial-wave method [7] and analytic resolution [6] in the CB approximation. The comparsions among the three kinds of calculated results are shown in Tables I and II, respectively. The present results are in good agreement with those obtained by the other two methods.

In conclusion, we showed that the Coulomb-Born theory with non-partial-wave analysis provides a powerful method to compute cross sections for the electron-impact excitation of a many-electron atomic ion system. From the viewpoint of methodology, our approach has the following distinguishing features: (a) For the practical application it should be emphasized that the appearance of the form factor with the harmonic function is of great significance because the most accurate multiconfiguration Hartree-Fock wave function can be used for the process calculation, if wanted. (b) All the calculations will be 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. Finally, we expect that our formalism will be able to open up vistas for the CB approximation.

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