Generalized Coulomb-projected Born-approximation cross sections for atomic excitation by charged-particle impact*

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An expression is given for the $(n_i, l_i = 0 \rightarrow n_f, l_f = 0)$ excitation cross section in terms of a single one-dimensional integral with the aid of a transformation to prolate spheroidal coordinates. Results are given for the $1s$-$2s$ excitation of arbitrary-Z hydrogenic targets. For our choice of wave functions the cross sections are found to scale as Z^{-4} at fixed $E_{\rm inc}/Z^2$. The principal difference between the Coulomb-projected Born-approximation (CPBA) and Born results is in the large-angle portion of the differential cross section. This, however, leads to CPBA and Born momentum-transfer cross sections which differ by less than 20% at high energies for $1s$-$2s$ transitions.

I. INTRODUCTION

Distorted-wave calculations are becoming more widely used in atomic-scattering theory, partially due to interest in plasmas where the presence of long-range electrostatic interactions suggests a need to include Coulomb distortion. Geltman and Hidalgo[1-5] have introduced a distorted-wave Born approximation (DWBA), the Coulomb-projected Born approximation (CPBA), which they have used to compute excitation and ionization cross sections for electrons on hydrogen and helium. Junker[6] has pointed out that the CPBA is a special case of a more general class of distorted-wave Born calculations and has applied this generalization to excitation of atoms by electron impact. Stauffer and Morgan[7,8] have used a generalized CPBA to calculate cross sections for the excitation of sublevels of hydrogen. In the case of excitation, the distorted-wave calculations of Geltman and Hidalgo, Junker, and Stauffer and Morgan retain some of the characteristic simplicity of the Born approximation.

In this paper we use prolate spheroidal coordinates to reduce the number of numerical integrations necessary to compute the T matrix for atomic excitation in a generalized CPBA. We apply our method to the case of $(n_i, l_i = 0 \rightarrow n_f, l_f = 0)$ atomic excitation by a projectile of charge Z_a, where the atomic states are represented in terms of Slater orbitals. The transformation to prolate spheroidal coordinates allows us to express the T matrix in terms of a single one-dimensional integral. As an example we consider in detail the case of $1s$-$2s$ excitation of hydrogenic targets by electron impact, for which we discuss the dependence of the differential and total cross sections on the atomic number Z of the target in terms of a scaling relation in Z. We also present calculations of the momentum-transfer cross section. The momentum-transfer cross section is equal to the differential cross section multiplied by an angularly dependent weighting factor which increases with scattering angle (θ). Thus the CPBA is particularly well suited to determine momentum-transfer cross sections, since the Coulomb distortion included in the CPBA is most significant at large angles. Momentum-transfer cross sections are pertinent because they may be used to calculate certain plasma transport coefficients for processes such as diffusion and electrical conductivity.[9-11]

In Sec. II we summarize the theory giving the distorted-wave T matrix. In Sec. III we reduce the $1s$-$2s$ hydrogenic T matrix to a formula requiring no integrations. Sec. IV contains a discussion of the results obtained from the formula of Sec. III in terms of differential, momentum-transfer, and total cross sections, and a scaling relation in Z. In the Appendix we present the details of the reduction of the integrals. Atomic units will be used throughout except where otherwise specified.

II. THEORY

The Hamiltonian of a projectile of charge Z_a with momentum $\vec{k}_0$ which is interacting with an atomic system of nuclear charge Z_b containing n electrons may be written as

$$H = H_0 + V_0 = H_0 + U + W, \tag{1}$$

where

$$H_0 = -\frac{1}{2\mu}\nabla_a^2 + \sum_{i=1}^{n}\left(-\frac{1}{2}\nabla_i^2 - \frac{Z_b}{r_i} + \frac{1}{2}\sum_{j\neq i}^{n}\frac{1}{r_{ij}}\right),$$

$$U = \frac{Z_a Z_b}{R}, \quad W = \sum_{i=1}^{n}\frac{-Z_a}{r_{ia}}.$$

The transition matrix element T_{if} may be expanded as[12]

$$T_{if} = \langle \chi_f^- | V_0 - W | \phi_i \rangle + \langle \chi_f^- | W | \Psi_i^+ \rangle \tag{2a}$$

$$= \langle \chi_f^- | \frac{Z_a Z_b}{R} | \phi_i \rangle + \langle \chi_f^- | \sum_{j=1}^{n}\frac{-Z_a}{r_{ja}} | \Psi_i^+ \rangle, \tag{2b}$$

where the eignefunctions ϕ_i, χ_f, Ψ_i^+ are defined as

$$H_0\phi_i = E\phi_i, \quad (H_0+U)\chi_f = E\chi_f, \quad (H_0+V_0)\Psi_i = E\Psi_i, \tag{3}$$

and satisfy the appropriate boundary conditions.

The first term in T_{if} can be shown to vanish since the perturbation U depends only on the relative separation of the centers of mass of the target and projectile. In the case of a hydrogenic target the distorted wave χ_f^- is exactly known and is simply a product of a Coulomb wave function and a hydrogenic wave function if exchange is neglected when the projectile is an electron. In general, χ_f^- may be written as

$$\chi_f^- = \chi_{Z_a Z_b}^-(\vec{k}_f, \vec{R})\chi_f(\vec{r}_1, \ldots, \vec{r}_n)$$

where $\chi_{Z_a Z_b}^-$ is a Coulomb wave function[13] of charge parameter $Z_a Z_b$ and $\chi_f(\vec{r}_1, \ldots, \vec{r}_n)$ is the final-state atomic wave function. Again exchange has been neglected if the projectile is an electron. If $\chi_f(\vec{r}_1, \ldots, \vec{r}_n)$ is approximated by a variational configuration-interaction (CI) or self-consistent-field (SCF) wave function constructed from Slater or hydrogenic orbitals, the results in the Appendix can be used to compute the integrals required to evaluate Eq. (2b).

If in addition one neglects the interaction between the active electron and the rest of the electrons in the target, χ_f^- may be approximated by

$$\chi_f^- = \chi_{Z_a Z_b}^-(\vec{k}_f, \vec{R})U_{Z_c^*}(\vec{r}_b)\Gamma_f(\vec{r}_1, \ldots, \vec{r}_{n-1}) \tag{4a}$$

where $U_{Z_c^*}$ is a bound-state wave function of effective charge Z_c^*, and Γ_f represents the undisturbed atomic electrons.

In the normal Born approximation Ψ_i^+ is expanded in terms of plane waves, but as has been previously discussed[6] Ψ_i^+ can be expanded in terms of Coulomb waves of charge-parameter δ, so that, retaining only the first-order term,

$$\Psi_i^+ \approx \chi_\delta^+(\vec{k}_0, \vec{R})U_{Z_b^*}(\vec{r}_b)\Gamma_i(\vec{r}_1, \ldots, \vec{r}_{n-1}), \tag{4b}$$

where the bound electrons have been approximated as in Eq. (4a).

The transition matrix element may now be written as

$$T_{if}^{\mathrm{DWBA}} = \langle \chi_{Z_a Z_b}^- U_{Z_c^*}\Gamma_f | \sum_{j=1}^{n}\frac{-Z_a}{r_{ja}} | \chi_\delta^+ U_{Z_b^*}\Gamma_i \rangle. \tag{5}$$

If in addition, $U_{Z_c^*}$ is orthogonal to $U_{Z_b^*}$, then

$$T_{if}^{\mathrm{DWBA}} = \langle \chi_{Z_a Z_b}^- U_{Z_c^*} | -Z_a/r_a | \chi_\delta^+ U_{Z_b^*} \rangle, \tag{6}$$

where the assumption is made that $\Gamma_i = \Gamma_f$. It has been pointed out[14-16] that it is not necessary to require $\Gamma_i = \Gamma_f$ as long as a sum over the probability of scattering into all final states Γ is understood. For $\delta = 0$ this approximation reduces to the CPBA of Geltman and Hidalgo.

III. APPLICATION

In the case of an $l_i = l_f = 0$ atomic target the reduction of the expression for T_{if}^{DWBA} to a one-dimensional integral is given in the Appendix. In this section and the following one we will be concerned with the special case of $1s$-$2s$ excitation of a hydrogenic target by electron impact. We have chosen $\delta = 0$ so that our initial incoming wave becomes a plane wave, and our calculation therefore reduces to the CPBA. The initial and final wave functions then become[17]

$$\chi_{\delta\to 0}^+\psi_{1s} = (Z_b^{3/2}/\sqrt{\pi})e^{i\vec{k}_0\cdot\vec{R}}e^{-Z_b r_b}, \tag{7a}$$

$$\chi_{Z_a Z_b}^-\psi_{2s} = (Z_b^{3/2}/2\sqrt{2\pi})(1 - Z_b r_b/2)e^{i\vec{k}_f\cdot\vec{R}}e^{-\pi\alpha/2} \times \Gamma(1-i\alpha) \times {}_1F_1(i\alpha, 1, -i(k_f R + \vec{k}_f\cdot\vec{R}))e^{-Z_b r_b/2}, \tag{7b}$$

where $\alpha = Z_a Z_b/v_f$. If we substitute Eqs. (7a) and (7b) into Eq. (6), then T_{if}^{DWBA} becomes

$$T_{if}^{\mathrm{DWBA}} = C\int d\vec{r}\int d\vec{R}\, e^{i\vec{q}\cdot\vec{R} - \lambda r_b} r_a^{-1} \times {}_1F_1(-i\alpha, 1, i(k_f R + \vec{k}_f\cdot\vec{R})) \times (1 - Z_b r_b/2), \tag{8}$$

where

$$\vec{q} = \vec{k}_0 - \vec{k}_f, \quad \lambda = \tfrac{3}{2}Z_b,$$

$$C = (-Z_b^3 Z_a/2\pi\sqrt{2})e^{-\pi\alpha}\Gamma(1+i\alpha).$$

We can put T_{if}^{DWBA} in the convenient form

$$T_{if}^{\mathrm{DWBA}} = \frac{-Z_b^3 Z_a}{2\pi\sqrt{2}}e^{-\pi\alpha/2}\Gamma(1+i\alpha)\left(1 + \frac{Z_b}{2}\frac{\partial}{\partial\lambda}\right)I(\lambda, \vec{q}), \tag{9}$$

$$I(\lambda, \vec{q}) = \int d\vec{r}_b\int d\vec{R}\, e^{i\vec{q}\cdot\vec{R}} r_a^{-1} e^{-\lambda r_b} \times {}_1F_1(-i\alpha, 1, i(k_f R + \vec{k}_f\cdot\vec{R})).$$

The integration over $d\vec{r}_b$ is made easier by first transforming to prolate spheroidal coordinates[18] (see Appendix), and the resultant integral over $d\vec{R}$ is a simple case of the type of integral considered by Nordsieck,[19] so that we are left with the final expression for $I(\lambda, \vec{q})$[20]:

$$I(\lambda, \vec{q}) = \left(\frac{4\pi}{\lambda}\right)^2 \left(\frac{2}{\lambda} D + 2(E)(F)\right), \tag{10}$$

where

$$D = \frac{(k_0^2 - k_f^2)^{i\alpha}}{q^{2+2i\alpha}} - \frac{(k_0^2 - k_f^2 - 2i\lambda k_f + \lambda^2)^{i\alpha}}{(\lambda^2 + q^2)^{1+i\alpha}},$$

$$E = (\lambda^2 + q^2)^{-1-i\alpha}(k_0^2 - k_f^2 - 2i\lambda k_f + \lambda^2)^{i\alpha},$$

$$F = \frac{-(1+i\alpha)\lambda}{\lambda^2 + q^2} + \frac{i\alpha(\lambda - ik_f)}{k_0^2 - k_f^2 - 2i\lambda k_f + \lambda^2}.$$

With the above expression for T_{if}^{DWBA} we calculate the differential cross section given by

$$\frac{d\sigma}{d\Omega} = \frac{\mu^2 k_f}{4\pi^2 k_0} |T_{if}^{\mathrm{DWBA}}|^2. \tag{11}$$

The total cross section is calculated by numerically integrating the above expression. Note that for this special case, the results of which are presented in the next section, the T matrix can be calculated directly whereas in the case examined in the Appendix a one-dimensional integration is required.

IV. RESULTS

The expression derived in the previous section allows us to calculate the differential and total cross sections for $1s$-$2s$ excitation by electron impact of any hydrogenic target. We have considered the atomic number Z of the target as a variable and determined the cross sections for the isoelectronic sequence $H, He^+, Li^{++}, \ldots$. For the Born approximation there exists a scaling relation in Z, such that $Z^4\, d\sigma/d\Omega$ and $Z^4\sigma$ are independent of Z when calculated at the same value of scaled energy, $E_{\mathrm{scaled}} = E_{\mathrm{inc}}/|E_{2s} - E_{1s}| = E_{\mathrm{inc}}/(10.2\ \mathrm{eV})Z^2$. We have found that our CPBA differential and total cross sections scale in exactly the same fashion. This scaling relation is also satisfied by the differential and total momentum-transfer cross sections (which we define and discuss later) in both Born and CPBA calculations.[20] It should be noted that this simple scaling relation is dependent on our particular choice of hydrogenic wave functions[21] where we have chosen the same initial and final effective charge.

We now compare our CPBA results with those of the plane-wave Born approximation. In Fig. 1 we present the scaled Born and CPBA differential cross sections as a function of the scattering angle

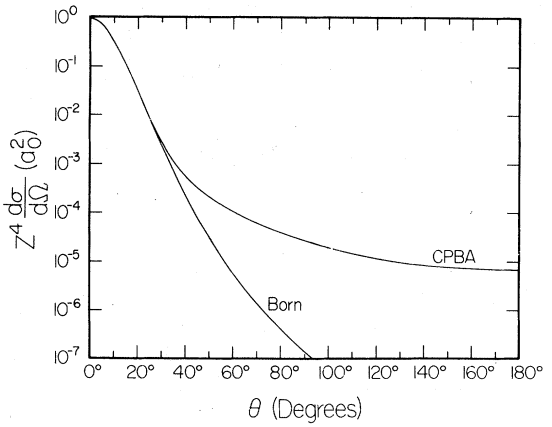

FIG. 1. CPBA and Born differential cross sections for $1s$-$2s$ excitation of hydrogenic (Z) targets by electron impact at $200Z^2$ eV.

θ at $200 \times Z^2$ eV electron-impact energy.[22] At small anges the two curves agree, but as θ increases the CPBA becomes several orders of magnitude larger than the Born curve. This wide angle behavior is explained[2] by noting that in the CPBA the projectile-nucleus interaction is included in H_0 thus taking into account the possibility of large-angle scattering off of the nucleus. Geltman and Hidalgo[2] have compared CPBA and Born differential cross sections to the $1s$-$2s, 2p$ data of Williams[23] and found that the data more closely follow the CPBA curve.

Despite the large differences between Born and CPBA angular distributions, the total cross sections are generally in agreement. This is shown in Fig. 2, which is a plot of $Z^4\sigma$ versus the scaled energy $E_{\mathrm{inc}}/|E_{2s} - E_{1s}|$. If we consider electrons on hydrogen ($Z = 1$), then for $E_{\mathrm{inc}} > 25$ eV the total cross sections agree to within 10%. This is due to

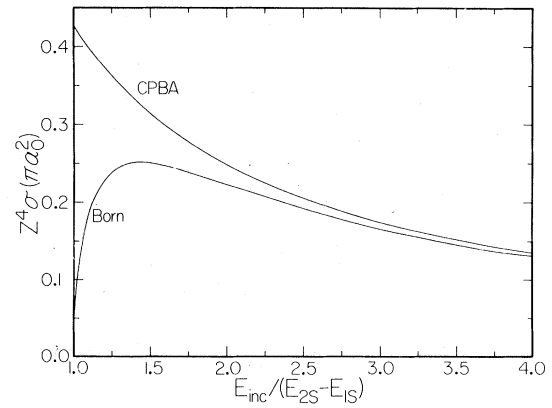

FIG. 2. Total Born and CPBA cross sections for $1s$-$2s$ excitation of hydrogenic targets by electron impact as a function of the scaled energy $E_{\mathrm{inc}}/|E_{2s} - E_{1s}|$.

the sharp drop off of $d\sigma/d\Omega$ with θ, as is shown in Fig. 1, so that most of the total cross section is summed up in the first few degrees where the two curves agree.

In order to accentuate the differences seen in Fig. 1, we consider the momentum-transfer cross section defined by

$$\frac{d\sigma_m}{d\Omega} = \left(1 - \frac{k_f}{k_0}\cos\theta\right)\frac{d\sigma}{d\Omega}. \tag{12}$$

This momentum-transfer cross section $d\sigma_m/d\Omega$ is equal to the change in the z component of momentum (normalized to k_0) times the differential cross section. It is clear that the effect of the $1-(k_f/k_0)\cos\theta$ term is to amplify $d\sigma/d\Omega$ at large angles. Thus we expect the momentum-transfer cross section to amplify the differences between CPBA and Born calculations. Momentum-transfer cross sections for excitation, ionization, and elastic scattering are used to define some plasma transport properties such as diffusion and electrical conductivity.[9-11] Our purpose here is to see whether the plane-wave Born excitation cross section, which is too small at large angles, is adequate for calculation of plasma transport properties.

In Fig. 3 we compare differential cross sections and momentum-transfer differential cross sections in the Born and CPB approximations at $100Z^2$ eV. Note that at small angles the important effect is the $1-(k_f/k_0)\cos\theta$ term while at large angles the greatest differences are due to Coulomb distortion. The total momentum-transfer CPBA and Born calculations displayed in Fig. 4 have the same shape and relative characteristics as the CPBA and Born total cross sections shown in Fig. 2. The large differences between CPBA and Born differential cross sections are not evident in the

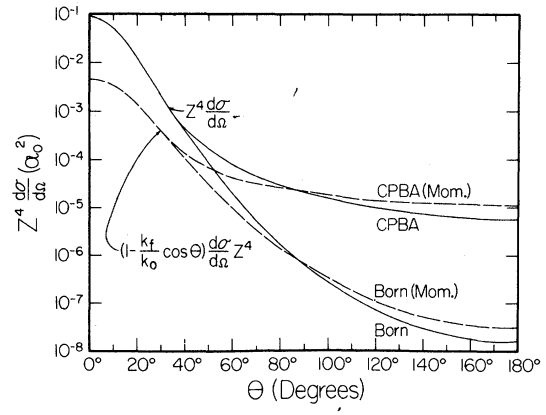

FIG. 3. CPBA and Born differential and momentum-transfer cross sections for $1s$-$2s$ excitation by electron impact of hydrogenic targets at $100Z^2$ eV.

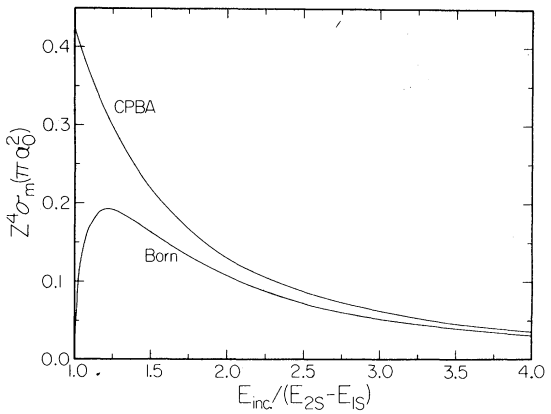

FIG. 4. Total Born and CPBA momentum-transfer cross sections for $1s$-$2s$ excitation of hydrogenic targets by electron impact as a function of the scaled energy $E_{\rm inc}/|E_{2s}-E_{1s}|$.

total cross sections.

Plasma transport coefficients depend on momentum-transfer cross sections which in turn are relatively sensitive to the differential cross section at large angles. As has been demonstrated the plane-wave Born approximation is often orders of magnitude too low at large angles, suggesting that use of these Born calculations for the plasma transport coefficients may lead to large errors. Our CPBA calculations on the other hand give a more reasonable estimate of the wide-angle distributions. By comparing momentum-transfer cross sections computed in the Born and CPBA approximations, one may estimate the error due to the use of the Born approximation in computing plasma properties. The CPBA Coulomb distortions affect both the total cross section and the momentum-transfer cross section. Consequently in Fig. 5 we compare the ratio $\sigma^{\rm CPBA}/\sigma^{\rm Born}$ for both total cross sections and momentum-transfer cross sections for $1s$-$2s$ excitation. The effect of the CPBA Coulomb distortions (reflecting large-angle contributions absent in Born calculations) on the

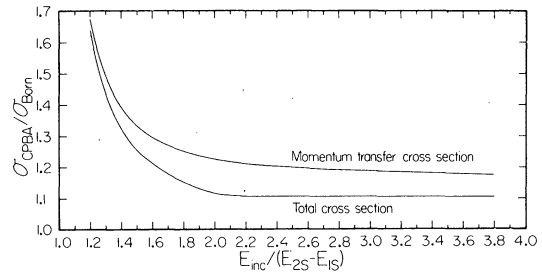

FIG. 5. Ratio of $\sigma^{\rm CPBA}/\sigma^{\rm Born}$ as a function of the scaled energy $E_{\rm inc}/|E_{2s}-E_{1s}|$ for both total cross sections and momentum-transfer cross sections.

momentum-transfer cross section is about 10% greater than the effect of Coulomb distortions on total cross sections. It should be noted that of all possible excitation and ionization cross sections contributing to plasma-transport properties, $1s$-$2s$ excitation is usually not a major contribution. Nevertheless, we feel that our $1s$-$2s$ excitation example is typical. Hence we suggest that error in momentum-transfer cross sections computed using plane-wave Born amplitudes, which are inadequate for wide-angle scattering, may be about 10%, i.e., not an order-of-magnitude effect.

APPENDIX

An appropriate linear combination of Slater orbitals may be used to express either hydrogenic or nonhydrogenic bound-state wave functions. We consider only $l_i = l_f = 0$. For simplicity of presentation we represent $U_Z(\vec{r}_b)$ as a single Slater orbital[24] of the form

$$U^{n00}_{Z_b}(\vec{r}_b) = N_n r_b^{n-1} e^{-Z_b r_b} Y_0^0(\hat{r}_b), \tag{A1}$$

where

$$N_n = [(2Z_b)^{2n+1}/(2n)!]^{1/2}.$$

The Coulomb wave functions have the form[13]

$$\chi^-_{Z_a Z_b} = e^{-\pi\alpha_f/2}\Gamma(1 - i\alpha_f) e^{i\vec{k}_f\cdot\vec{R}} \times {}_1F_1(i\alpha_f, 1, -i(k_f R + \vec{k}_f\cdot\vec{R})),$$

$$\chi^+_\delta = e^{-\pi\alpha_i/2}\Gamma(1 + i\alpha_i) e^{i\vec{k}_i\cdot\vec{R}} \times {}_1F_1(-i\alpha_i, 1, i(k_i R - \vec{k}_i\cdot\vec{R})),$$

where

$$\alpha_f = Z_a Z_b/v_f, \quad \alpha_i = \delta/v_i,$$

so that Eq. (6) becomes

$$T^{\mathrm{DWBA}}_{if} = -\int d\vec{R} \int d\vec{r}_b\, N_{n_i} N_{n_f} F(\vec{R})(Z_a/r_a) \times r_b^{n_i+n_f-2} e^{-\lambda r_b}(1/4\pi), \tag{A2}$$

$$F(\vec{R}) = e^{i\vec{q}\cdot\vec{R}} e^{-\pi(\alpha_i+\alpha_f)/2}\Gamma(1 + i\alpha_i)\Gamma(1 + i\alpha_f) \times {}_1F_1(-i\alpha_i, 1, i(k_i R - \vec{k}_i\cdot\vec{R})) \times {}_1F_1(-i\alpha_f, 1, i(k_f R + \vec{k}_f\cdot\vec{R})),$$

$$\vec{q} = \vec{k}_i - \vec{k}_f, \quad \lambda = Z_b^* + Z_c^*$$

with Z_b^* and Z_c^* as the effective initial and final nuclear charges. We then make the transformation to prolate spheroidal coordinates[18] given by

$$r_a = \tfrac{1}{2}R(\xi + \eta), \quad r_b \sin\theta_b = \tfrac{1}{2}R[(\xi^2 - 1)(1 - \eta^2)]^{1/2},$$
$$r_b = \tfrac{1}{2}R(\xi - \eta), \quad r_b\cos\theta_b = \tfrac{1}{2}R[\xi\eta - 1], \tag{A3}$$
$$d\vec{r}_b = \tfrac{1}{2}R\, r_a r_b\, d\xi\, d\eta\, d\phi_b,$$
$$1 \le \xi \le \infty, \quad -1 \le \eta \le 1, \quad 0 \le \phi_b \le 2\pi,$$

so that the T matrix becomes

$$T_{if} = A\int d\vec{R}\, F(\vec{R})(R/2)^{n_i+n_f} \times \int\int d\eta\, d\xi\, e^{-\lambda R(\xi-\eta)/2}(\xi - \eta)^s, \tag{A4}$$

where

$$A = -\tfrac{1}{2} Z_a N_{n_i} N_{n_f}, \quad s = n_i + n_f - 1.$$

We perform a binomial expansion on $(\xi - \eta)^s$:

$$(\xi - \eta)^s = \sum_{j_1=0}^{s} \binom{s}{j_1} (-1)^{j_1}\eta^{j_1}\xi^{s-j_1}. \tag{A5}$$

Substituting (A5) into (A4) yields

$$T_{if} = A\sum_{j_1=0}^{s}\binom{s}{j_1}(-1)^{j_1} \times \int_{-1}^{1} d\eta\,\eta^{j_1}\int d\vec{R}\, F(\vec{R})(R/2)^{n_i+n_f} e^{+\lambda R\eta/2} \times \int_1^\infty d\xi\, e^{-\lambda R\xi/2}\xi^{s-j_1}.$$

With $\omega = \lambda R/2$ we have for the ξ integral:

$$\int_1^\infty d\xi\, e^{-\omega\xi}\xi^{s-j_1} = (-1)^{s-j_1}\left(\frac{d}{d\omega}\right)^{s-j_1}\int_1^\infty d\xi\, e^{-\omega\xi} = (-1)^{s-j_1}\left(\frac{d}{d\omega}\right)^{s-j_1}\frac{e^{-\omega}}{\omega} = \sum_{j_2=0}^{s-j_1}\binom{s-j_1}{j_2}(j_2)!\,\frac{e^{-\omega}}{\omega^{j_2+1}}. \tag{A6}$$

The resultant integral over $\vec{R}$ can be written in the form:

$$\int d\vec{R}\, F(\vec{R})(R/2)^{n_i+n_f}(\lambda R/2)^{-1-j_2}e^{-\lambda R(1-\eta)/2} = G(\alpha_i, \alpha_f)\left(\frac{d}{du}\right)^{n_i+n_f-j_2} \times \int \frac{d\vec{R}}{R} e^{-uR + i\vec{q}\cdot\vec{R}}\, {}_1F_1(-i\alpha_i, 1, i(k_i R - \vec{k}_i\cdot\vec{R})) \times {}_1F_1(-i\alpha_f, 1, i(k_f R + \vec{k}_f\cdot\vec{R})),$$

where

$$G(\alpha_i, \alpha_f) \equiv \frac{\lambda^{-1-j_2}}{2^{n_i+n_f-1-j_2}}(-1)^{n_i+n_f-j_2} \times \Gamma(1 + i\alpha_i)\Gamma(1 + i\alpha_f)e^{-\pi(\alpha_i+\alpha_f)/2} \tag{A7}$$

and $u = \tfrac{1}{2}\lambda(1 - \eta)$.

The $\vec{R}$ integral is now in the form considered by Nordsieck,[19] so that

$$\int d\vec{R}\,\frac{e^{-uR+i\vec{q}\cdot\vec{R}}}{R}\,{}_1F_1(-i\alpha_i,1,i(k_iR-\vec{k}_i\cdot\vec{R}))$$

$$\times\,{}_1F_1(-i\alpha_f,1,i(k_fR+\vec{k}_f\cdot\vec{R}))$$

$$=2\pi e^{\pi\alpha_i}g_1^{-i\alpha_i-1}g_2^{i(\alpha_i-\alpha_f)}(g_2+g_3)^{i\alpha_f}$$

$$\times\,{}_2F_1\left(1+i\alpha_i,-i\alpha_f,1,\frac{g_1g_3-g_4g_2}{g_1(g_2+g_3)}\right)$$

$$\equiv 2\pi e^{\pi\alpha_i}J(u,\vec{q}), \qquad \text{(A8)}$$

$g_1\equiv\frac{1}{2}(q^2+u^2)$, $g_2\equiv\vec{k}_i\cdot\vec{q}+iuk_i-g_1$

$g_3\equiv k_ik_f+\vec{k}_i\cdot\vec{k}_f-g_4$, $g_4\equiv\vec{k}_f\cdot\vec{q}-iuk_f$.

Thus the final expression for T_{if} can be written as

$$T_{if}=B\sum_{j_1=0}^{s}\sum_{j_2=0}^{s-j_1}\binom{s}{j_1}\binom{s-j_1}{j_2}(-1)^{j_1-j_2}\left(\frac{2}{\lambda}\right)^{j_2}(j_2)!$$

$$\times\int_{-1}^{1}d\eta\,\eta^{j_1}\left(\frac{d}{du}\right)^{n_i+n_f-j_2}[J(u,\vec{q})], \qquad \text{(A9)}$$

where

$$B=Z_a(-1)^{n_i+n_f+1}e^{-\pi(\alpha_f-\alpha_i)/2}$$

$$\times\,\Gamma(1+i\alpha_f)\Gamma(1+i\alpha_i)\pi 2^{+1-n_i-n_f}\lambda^{-1}N_{n_i}N_{n_f},$$

$$N_n=[(2Z)^{2n+1}/(2n)!\,]^{1/2},$$

$$\lambda=Z_b^*+Z_c^*,\quad u=\tfrac{1}{2}\lambda(1-\eta),$$

and with $J(u,\vec{q})$ defined by Eq. (A8). Note that generalization of the above technique to include nonzero angular-momentum states requires the introduction of a rotation operator.

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