Correction of a relativistic impulse approximation expression used to obtain Compton profiles from photon scattering doubly differential cross sections

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Abstract
A Compton profile (CP) can provide useful information about the electron populations and distributions in atoms, molecules, and ions to assess many physical properties of matter. However, a CP cannot be measured directly, but must be obtained from scattering data. The CPs discussed in this study are derived from photon-atom doubly differential cross sections (DDCS) via the following expression which is derived from an impulse approximation (IA) theory given by \( \text{DDCS} = KJ \), where \( K \) represents a kinematic factor and \( J \) represents the CP. A relativistic version of this expression (i.e., RKJ)—an approximation of the full relativistic IA expression—is used for relativistic regimes; however, it does not yield accurate results for the inner and middle shells of moderate to heavy atoms. In this study, expressions from nonrelativistic (NR) hydrogen-like wavefunctions with a relativistic QED kinematic factor \( K_{\text{rel}} \) and relativistic electron energy were derived to correct the RKJ expression for the K, L, M, and N atomic subshells. This derivation made it possible for relativistic contributions and screening effects to largely cancel, for any regime of energy angle and \( Z \). Thus, the RKJ error which can be greater than 30% is reduced to within few percent over 99% of the electron momentum distribution range of any subshell CP when compared to published tabulated theoretical values. Two simple versions of the relativistic QED kinematic component of the corrected RKJ expressions were obtained and tested: one valid at high photon energies, and the other at small scattering angles. RKJ corrections were applied to the extraction of CP from the full spectrum K-N shell DDCS, which resulted in much improved accuracy for the K-shell. Good agreement was observed with tabulated beyond K-shell CPs around the tail regions, but systematic differences were found to occur at the maxima. The details of this phenomenon are illustrated and discussed in this article.

1. Introduction
There are numerous applications for Compton profiles (CP). They can be used to assess electronic properties of atoms, molecules and ions that make-up all phases of matter. Applications of CP transcend nearly all branches of physical science as well as some aspects of medicine. Because CP can only be obtained indirectly from scattering data, expressions derived from impulse approximations (IAs) are typically used to obtain CPs from such data. However, there are many instances under which such expressions break down. Up until now, this problem has not been resolved, which is the purpose for the present study.

A simple method based on relativistic impulse approximation (IA), which can be used to obtain more accurate entire-atom Compton profiles (CP), especially around the tail region, from Compton photon scattering doubly differential cross sections (DDCS), is proposed in this paper. In nonrelativistic (NR) regimes (low energy and small electron binding energies), the expression \( \text{DDCS} = KJ \), where \( J \) represents the CP and \( K \) represents a kinematic factor providing accurate values for the CP when it is obtained from DDCS. However, in relativistic regimes, this expression is replaced by an expression with the same form but an approximation of the
full relativistic IA (RIA) expression for photon atom DDCS. Ribberfors [1], Eisenberger and Reed [2], and Manninen [3] implied that this expression can be used instead of the full RIA expression under most circumstances. In this work, we found that a factorizable expression becomes progressively less accurate with increasing binding energy $E_b$. In addition, the accuracy decreases with increasing orbital angular momentum quantum number $l$ within any given shell of an atom. The loss of accuracy is the most pronounced for inner shells of the heavy atoms. Spies and Bell suggested that the factorizable expression has limitations based on their study on the use of DDCS measured from proton scattering experiments to obtain a CP [4].

Ribberfors [1] attempted to correct the RKJ expression, which is still being used today. However, his corrected expression yields poor results, especially if one transforms a heavy atom inner shell Compton peak into a CP. This is because his expression was derived with the implicit assumption of a narrow Compton peak which corresponds to a small $E_b$. His expression would provide a zero RKJ error for back-angle scattering, while the present study reveals that this error is the greatest at that angle. The present RKJ correction provides large reductions of the RKJ error over all energies and scattering angles.

Some examples wherein the CP is obtained from measured DDCS in relativistic regimes and compared to theoretical CP have already been presented [4–7]. There has been continuing interest in the measurement and prediction of heavy atom CPs, partly because of advances in the Dirac equation–based electronic structure methods used to calculate the CP [5]. Also with the advent of high energy and high intensity synchrotron radiation sources, higher precision measurements can be made for even the heaviest atoms. This is why there is a greater need for more accurate values for CP obtained from the measured DDCS.

Theoretical calculations were used [6] for comparisons with CP obtained from measured DDCS [5]. When Sakurai [5] compared their entire atom Xenon CP to theoretical Dirac Hartree–Fock Xe CP they stated that ‘the 1s orbital should not be included in the summation. However this effect can be ignored for the present analysis at least around where $p_z = 0$ because 1s contributes only 0.15% of the total magnitude at the CP maximum.’ However the inner shell CPs do become progressively more significant as one goes to higher $p_z$ until they become dominant at the extremes. An improved method to transform measured scattering data into CP should dramatically improve the accuracy of experimentally derived CPs at the extremes.

Sakurai et al [5] also reported rather prominent differences around the CP maximum between published tabulated theoretical CPs and those derived from their experiments for Xe entire-atom CPs. Such differences may be due to beyond the electron momentum distribution function factors which are not accounted for in the theoretical methods to obtain the published CPs. However the effect does not appear to be so great that it would prevent one from using CP results to evaluate electron distributions and atomic shell populations in matter. There may be other factors that contribute to the deviations between theoretical and experimentally obtained CP such as electron correlation as well as experimental error. This issue which may be QED related is discussed in section 5 of this article.

It is desirable to obtain accurate CP values for the inner shell because its contribution is dominant in the extremes of the entire-atom Compton CP, wherein the RKJ error is the largest. One reason that the extrema of the CP is of current interest is that this anisotropic region contributes indirectly to the bonding properties of molecules and semiconducting materials, including those composed of heavy atoms. Inner shell states can have an influence although conductivity involves valence electrons. This can occur when such states are orthogonalized with valence states [8]. For example, [8–14] provide discussions on the measurement and prediction of CPs in the context of molecules and semiconducting materials.

IA is the most widely used theory for Compton scattering because it is simple in form (especially the NR version) and more directly related to relevant physical quantities; under the right circumstances, it provides fairly accurate predictions for the Compton peak region of the spectrum while requiring minimal computational resources. The IA theory does not produce a complete DDCS spectrum. Such a full spectrum includes an infrared rise (or divergence) and resonance. See [15, 16] for a detailed discussion of the full DDCS spectrum.

The IA theory is based on an assumption that the momentum and energy transfer from an incident photon to a target electron is sufficiently large such that electron binding effects can be neglected. Here, the bound states of an atom are treated as the momentum distribution of electrons in the absence of a potential. The final state of excited electrons can be approximated using a plane wave state. The IA theory works best for the prediction of the Compton peak region of the spectrum; the magnitude of the energy transfer is considerably greater than the binding energy of the ejected electron. This requirement can be considerably less restricted for DDCS than for triply differential cross sections (TDCS) [17].

NR expressions for DDCS can provide fairly accurate predictions for the DDCS of light atoms (see [18, 19]) if the incident photon energy is $\omega_i \ll m$ or $\theta \rightarrow 0^\circ$ [20]; otherwise, relativistic factors must be included (i.e., 7, 21–24) for examples. If there is a need to obtain a CP from DDCS in a relativistic regime, the most straightforward approach for Compton scattering is RKJ approximation, which is fairly accurate overall $\omega_i$ values; if the binding energy ($E_b$) is low, it becomes less accurate with increasing $E_b$. 


Although the RKJ error is the greatest for the K-shell, it is approximately 30% at the uranium K-shell CP peak maximum; the error persists for higher shells. The RKJ error at the 2s uranium CP peak maximum is approximately 6%, but it increases to approximately 15% for the 2p subshell. The RKJ error appears to be dependent on the angular momentum. For uranium, it is about 2% for 3s, 4% for 3p, 6% for 3d, and 3% for 4f. Then, it decreases monotonically from 2% for 4d to approximately 1% for the 4s CP. Around the CP maximum, outer shells contribute the most to the entire CP atom because the RKJ error remains significant, even for the 4f subshell of a heavy atom, wherein the correction of the RKJ error can significantly increase the accuracy of the entire atom CP when obtained from a DDCS spectrum. In addition, the RKJ error tends to be the smallest around the CP maximum, while it increases dramatically as one approaches the extremities. This is true for the entire-atom CP and for the single-subshell CP, but to a lesser degree. The method described in this article provides corrections to within a few percent error over at least 99% of the CP electron momentum distribution range when compared to theoretical electron wavefunction derived CP.

Expressions like those of the RKJ have been derived for other collision processes. Equation (4) in [4] and equation (16) in [23] for proton-atom and electron-atom collisions, respectively, are in the RKJ form. Such expressions can be used to obtain a CP from cross-sections in relativistic regimes. It seems quite likely that these expressions will have similar limitations when applied to bound electrons with high binding energies, wherein the RKJ expression can break down as the CP broadens. An RIA expression and its factorizable form is used in many branches of physics such as atomic, condensed matter, astro, nuclear, and subatomic particle physics.

The rest of this manuscript is organized as follows: in section 2, the relevant expressions for obtaining DDCS from non-relativistic and relativistic theories are provided, followed by an explanation of the cause of the RKJ error. The corrected RKJ expressions based on NR Coulombic wave functions—but with relativistic kinematic terms—are derived for the K, L, M, and N shells. The success of such an approach requires the substantial cancelation of relativistic and screening effects.

An analysis of the limitations of RKJ approximation based on the results of numerical calculations is described in section 3. Further, simpler expressions that can be used to correct RKJ in the small \( \omega_i \) and high \( \omega_f \) regimes are derived.

The \( Z \) dependence of the RKJ error at the CP maximum is given for various subshells at \( \theta = 180^\circ \) in section 4. The full RKJ correction was tested over a broad range of bound electron momenta, energies, and scattering angles for K, L, M, and N shell CPs. A comparison is drawn to identify how well each of the three expressions, the most general expression based on the relativistic QED kinematic expressions given by equation (5) in [1], and the small \( \theta \) and large \( \omega_f \) limits of the former expression, correct the RKJ error for the computations of K and L subshell CPs.

The validity of IA is presented in section 5 [15]. For test calculations, full DDCS spectra are calculated for K-N shells of some moderate to heavy atoms using the S-matrix QED code reported by Bergstrom et al [16]. These DDCSs are converted to CP using the RKJ correction method; the results are compared with those of established CP values obtained by Biggs et al [26]. The CP values were obtained by Biggs et al using Fourier-transformed Dirac large and small component wavefunctions. This provides a good standard for assessing the accuracy of CP extracted from both the S-Matrix and RIA DDCS because these CPs were obtained without the use of IA. Systematic differences between the S-Matrix and Biggs beyond the K-shell CP were found to occur around the CP maximum, while fair to good agreement resulted for those CP around the tail regions.

Finally, the conclusions are provided in section 6.

2. Theory

2.1. Nonrelativistic expressions for DDCS and Compton profiles

The NRIA formula for DDCS is expressed as the product of a kinematic factor \( K \) and CP \( f \) for a given \( n l \) quantum state.

\[
DDCS = \frac{d^2\sigma}{d\omega_id\Omega_f} = K_{NR}\rho_{NR}^{nl}(p_f), \quad (1)
\]

where \( \omega_i \) and \( \omega_f \) represent the incident and scattered photon energies, respectively; and \( \Omega_f \) represents the solid angle of the scattered photon. The expression for the NR CP \( f_{NR}^{nl} \) which is spherically symmetric, is given by

\[
f_{NR}^{nl}(p_f) = 2\pi \int_{|p|}^{\infty} p\rho_{NR}^{nl}(p)\,dp, \quad (2)
\]

where \( \rho(p) \) represents the electron momentum distribution function. The analytic Coulombic NR expression for the K-shell CP is given by
where $\rho_{NR}^{nl}$ is obtained from the NR Fourier transformed electron wavefunctions for a given $n$ and $l$ quantum state. The expression for $J_{NR}^{s}$ is obtained from a Coulombic K-shell NR electron momentum distribution function $\rho_{NR}^{s}$. $p_z$ denotes the component of the bound state electron momentum along the scattering vector, which is considered the $z$-axis by the convention. This equation is given by

$$p_z = \frac{(\omega_l - \omega_f)m}{|k|} - \frac{|k|}{2},$$

where the magnitude of the physical momentum transfer is given by

$$|k| = |k_i - k_f| = [\omega_i^2 + \omega_f^2 - 2\omega_i\omega_f \cos \theta]^1/2,$$

where $k_i$ and $k_f$ represent the momentum vectors of the incident and scattered photon, respectively. The kinematic factor $K_{NR}$ is given by

$$K_{NR} = \frac{r_0 m \omega_f X^{NR}}{2\omega_i|k|},$$

where $r_0$ and $\theta$ denote the classical electron radius and photon scattering angle, respectively, and

$$X^{NR} = 1 + \cos^2 \theta.$$

### 2.2. Relativistic expressions for DDCS and Compton profile

The full RIA expression for DDCS [1] is

$$\frac{d^2\sigma}{d\omega_f d\Omega_f} = \frac{r_0^2 \pi m^2 \omega_f}{2|k_i|} \int_{|p_{min}|}^{\infty} \rho_{rel}^{nlj}(p) X^{nlj}(\theta, \phi, p) dp,$$

where

$$E(p) = (p^2 + m^2)^{1/2},$$

is the initial bound state relativistic electron energy associated with the momentum component $p$. Here the units $c = \hbar = 1$ as well as $m = 1/\alpha$ applies throughout. $p_{min}$ represents the relativistic version of $p$, which is the minimum electron momentum required to cause Compton scattering at a given $\omega_i$, $\omega_f$, and $\theta$; it is given by

$$p_{min} = \frac{1}{|k|}[E(p_{min}) - \omega_i(1 - \cos \theta)].$$

Here, $E(p_{min}) = (p_{min}^2 + m^2)^{1/2}$ denotes the initial state electron energy associated with $p_{min}$, whereas $\rho_{rel}^{nlj}(p)$ is obtained from the Fourier transform of the relativistic large and small component wavefunctions for a given nlj quantum state. $\rho_{rel}$ is given by

$$\rho_{rel}^{nlj}(p) = G_{nlj}(p) + F_{nlj}(p).$$

Formulas for the Fourier transformed K-shell large and small component wavefunctions are given in appendix A.

The relativistic QED kinematic factor $X^{nlj}(\omega, \phi, p)$ is given as the integral over the azimuthal angle of the initial electron $\phi$ for the integrand $X^{nlj}(\omega, \theta, p, \phi)$ (equation B.64 in appendix B).

$$X^{nlj}(\omega, \theta, p) = \frac{1}{2\pi} \int_0^{2\pi} X^{nlj}(\omega, \theta, p, \phi) d\phi$$

$$= 2 + F\left[\frac{1}{U^{1/2}} \frac{1}{V^{1/2}}\right] + \frac{m^2}{\omega_i^2} \left[\frac{E - D}{U^{3/2}} + \frac{E - W - D}{U^{1/2}}\right]$$

$$F = W - 2m^2 \omega_i - 2m^4 \omega_i^2 W^2,$$

$$W = \omega_f(1 - \cos \theta),$$

$$D(p) = \frac{1}{|k|^2} (\omega_i - \omega_f \cos \theta)[E(p)(\omega_i - \omega_f) - \omega_i \omega_f (1 - \cos \theta)],$$

$$U(p) = [E(p) - W - D(p)]^2 - H^2(p),$$

$$V(p) = [E(p) - D(p)]^2 - H^2(p).$$
\[ H(p) = \frac{1}{|\mathbf{k}|} \omega f \sin \theta (p^2 - p_{\text{min}}^2)^{1/2}. \] (18)

The NR limit of \( X^{rel}(\omega, \theta, p) \), which is \( X^{NR}(\theta) = 1 + \cos^2 \theta \), results when \( \omega \ll m \) and/or as \( \theta \to 0^\circ \); see equation (25) in [20]. The form of equation (12) integrated over \( p \) and \( \phi \) is given in appendix C.

If the binding energy \( E_b \) is small, both \( X^{rel}(\omega, \theta, p) \) and \( E(p) \) in equation (8) become effectively constant with respect to \( p \) such that \( p \approx p_{\text{min}} \). Both can be factored out of the integral because of this assumption. The result is an expression that will be referred to in this article as RKJ approximation. This expression is

\[
\text{DDCS}^{rel} = \frac{d^2\sigma}{d\omega_f d\Omega_f} \approx K_{rel}(\omega, \theta, p_{\text{min}}) \int_{p_{\text{min}}}^{\infty} \rho_{rel}(p) dp = K_{rel}(\omega, \theta, p_{\text{min}}) J_{rel}(p_{\text{min}}). \] (19)

This expression has the same factorizable form as the NR expression given by equation (1). Here,

\[
K_{rel}(\omega, \theta, p_{\text{min}}) = C X^{rel}(\omega, \theta, p_{\text{min}}) / E(p_{\text{min}}) \] (20)

and

\[
C = \frac{r_0^2 \pi m^2 \omega_f}{2|\mathbf{k}|}. \] (21)

An important advantage of the RKJ approximation over the full RIA expression (8) is the relativistic CP, which is spherically symmetric and given by

\[
I_{njl}^{rel}(p_{\text{min}}) = \int_{p_{\text{min}}}^{\infty} \rho_{rel}^{nlj}(p) dp, \] (22)

can be obtained directly. An explicit formula for the fully relativistic K-shell CP is given in appendix D.

Ribberfors obtained the RKJ expression for all atomic subshells by integrating equation (8) by parts [1], which resulted in

\[
\text{DDCS}^{rel} = \frac{d^2\sigma}{d\omega_f d\Omega_f} = C \left[ \frac{J_{rel}(p_{\text{min}})X^{rel}(\omega, \theta, p_{\text{min}})}{E(p_{\text{min}})} + I_1 + I_2 \right], \] (23)

where the first term in the above expression is the RKJ approximation. It becomes valid if \( I_1 \) and \( I_2 \) are smaller than \( J_{rel}X^{rel}/E \). Expressions for \( I_1 \) and \( I_2 \) are given by

\[
I_1 = \int_{p_{\text{min}}}^{\infty} J_{rel}(p) \left( \frac{dX^{rel}(\omega, \theta, p)}{dp} \right) F(p) dp, \] (24)

and

\[
I_2 = \int_{p_{\text{min}}}^{\infty} J_{rel}(p)X^{rel}(\omega, \theta, p) F(p) dp, \] (25)

where \( dX^{rel}(\omega, \theta, p)/dp \) in \( I_1 \) is

\[
\frac{dX^{rel}}{dp}(\omega, \theta, p) = P \left[ -F \left( \frac{(AG - B)}{V^{3/2}} \right) + \frac{(AG - B)}{V^{3/2}} + \frac{m^4}{\omega_f^4} \left( \frac{A}{|\mathbf{k}|^2 E} \right) \left( U^{-3/2} + V^{-3/2} \right) \right. \]

\[
\left. + 3 \left( \frac{(AL - B)}{V^{3/2}} \right) + \frac{(AG - B)}{U^{3/2}} \right] \right), \] (26)

\[
A = \omega_f (\omega_i + \omega_f)(1 - \cos \theta), \] (27)

\[
B = (\omega_f \sin \theta) / |\mathbf{k}|, \] (28)

\[
G(p) = E(p) - W - D(p), \] (29)

\[
L(p) = E(p) - D(p)|/|\mathbf{k}|^2 E(p). \] (30)

### 2.3. Ribberfors attempt to obtain simple expressions to correct the RKJ approximation

Equation (23) is a mathematical identity, and it is possible to correct the RKJ expression using numerical methods. However, it remains a challenge even with the current computational resources. The first one requires fully relativistic Fourier transformed wavefunctions with the proper inclusion of electron–electron interactions. Then, we integrate twice over \( p \) for both \( I_1 \) and \( I_2 \). In addition, the integration over \( X^{rel} \) in \( I_2 \) and even more so for the integration over \( dX^{rel}/dp \) in \( I_1 \) can cause one to encounter singularities over some values of \( \omega_{\text{min}}, \omega_f \), and \( \theta \). This makes it impossible to obtain a corrected CP over its full range of \( p_{\text{min}} \).
Ribberfors was aware of difficulties involved in computing $I_1$ and $I_2$. Therefore, in his paper [1], he provided a simplified approach to correct the RKJ approximation. He initiated this by solving equation (23) for $J_{\text{rel}}$, which results in

$$J_{\text{rel}}(p_{\text{min}}) = \frac{\Delta_1(\omega, \theta, p_{\text{min}})}{I_{\text{rel}}(\omega, \theta, p_{\text{min}})} - \frac{\Delta_2(\omega, \theta, p_{\text{min}})}{I_{\text{rel}}(\omega, \theta, p_{\text{min}})}.$$

(31)

Here, Ribberfors assumed that $I_2$ is negligible (see equation (53) in [1]). He based his assumption on the presence of $E^2$ in the denominator of the integrand in equation (25), which is a relatively large value. Next, he simplified the formula for $dX_{\text{rel}}/dp$ by assuming that $E \approx m$, along with some other assumptions, which implicitly assume a narrow Compton peak. According to his formula (see [1], equation (52)), when $\theta = 180^\circ$, $I_1$ goes to zero, and this leads to the conclusion that the RKJ approximation is virtually exact at this angle. However, if we derive the derivative without considering any assumptions (see equation (26)–(30)), $I_1$ has the maximum value at $\theta = 180^\circ$. Further, $I_2$ is significant; it increases with an increase in electron $E_p$. Ribberfors was apparently not aware of the relationship between the increasing ejected electron binding energy, the subsequent broadening of the Compton peak, and the resulting increase in the RKJ error.

2.4. Simple analytic expressions to correct the RKJ formula based on nonrelativistic hydrogen like wavefunctions with relativistic kinematic factors $X_{\text{rel}}$, $dX_{\text{rel}}/dp$, and $E(p)$

A considerably better approach for obtaining a CP from the Compton peak of a DDCS spectrum is to rearrange equation (23) to yield

$$J_{\text{rel}}(p_{\text{min}}) = \frac{[1 - \Delta_1(\omega, \theta, p_{\text{min}}) - \Delta_2(\omega, \theta, p_{\text{min}})]DDCS_{\text{rel}}(\omega, \theta, p_{\text{min}})}{K_{\text{rel}}(\omega, \theta, p_{\text{min}})},$$

(32)

where

$$\Delta_1 = \frac{C_1}{DDCS_{\text{rel}}}$$

(33)

and

$$\Delta_2 = \frac{C_2}{DDCS_{\text{rel}}}$$

(34)

represent the corrections to the RKJ expression, whose values are relative to the magnitude of DDCS. Therefore, the values of $\Delta_1$ and $\Delta_2$ are on the order of unity. The advantages of expressing the corrected RKJ expression in this manner is that it allows relativistic and screening effects to largely cancel. This is because of the presence of similar factors in the integrands of numerators and denominators of $\Delta_1$ and $\Delta_2$ (see equations (8), (24) and (25)).

Another advantage is that the adverse effects of factoring $X_{\text{rel}}$, $dX_{\text{rel}}/dp$, and $E$ is minimized. The following equations illustrate how partial cancellations can occur.

$$\Delta = \int_{p_{\text{min}}}^{\infty} \frac{J_{\text{rel}}(p)X_{\text{rel}}(\omega, \theta, p)dp}{E(p)} \approx \int_{p_{\text{min}}}^{\infty} \frac{X_{\text{rel}}(\omega, \theta, p)dp}{E(p)} \int_{p_{\text{min}}}^{\infty} J_{\text{rel}}(p)dp = \int_{p_{\text{min}}}^{\infty} \frac{J_{\text{rel}}(p)dp}{E(p)}$$

(35)

$$\Delta = \frac{1}{p} \int_{p_{\text{min}}}^{\infty} \frac{J_{\text{rel}}(p)dp}{E(p)} \approx \frac{1}{p} \int_{p_{\text{min}}}^{\infty} \frac{X_{\text{rel}}(\omega, \theta, p)dp}{E(p)} \int_{p_{\text{min}}}^{\infty} \rho_{\text{rel}}(p)dp = \int_{p_{\text{min}}}^{\infty} \frac{J_{\text{rel}}(p)dp}{E(p)}$$

(36)

where $T = \frac{1}{p} \int_{p_{\text{min}}}^{\infty} \frac{J_{\text{rel}}(p)dp}{E(p)}$.

The resulting DDCS Compton peak is narrow when the binding energy ($E_b$) of the ejected electron is small for any given Compton ionization. This causes relevant upper and lower integration limits in equations (8), (24) and (25) to be very close in value. Therefore, one can justify factoring the kinematic functions of corresponding integrals for these three equations, while treating them as though they are constant with respect to the electron momentum $p$. However, when $E_b$ is large, the Compton peak is broad as is the case for electrons in the inner and middle shells of moderate to heavy atoms. Here, the relevant upper and lower integration limits differ greatly in value. Therefore, the factorization of the kinematic functions is not justified unless the resulting adverse effects are allowed to largely cancel. Such a cancelation is possible for the RKJ correction factors $\Delta_1$ and $\Delta_2$.

If the cancelations discussed for $\Delta_1$ and $\Delta_2$ illustrated in equations (35) and (36) are valid, one can use hydrogen-like NR wave functions instead of full Dirac large and small component wavefunctions. This leads to
\[
\Delta_1 \approx \frac{\int_{p_{\min}}^{\infty} J_{\text{rel}}(p) dp}{E^2(p_{\min}) J_{\text{rel}}(p_{\min})} \approx \frac{\int_{p_{\min}}^{\infty} J_{\text{NR}}(p) dp}{E^2(p_{\min}) J_{\text{NR}}(p_{\min})} = \Delta_{1\text{NR}}
\]
and
\[
\Delta_1 \approx \frac{T(\omega, \theta, p_{\min}) \int_{p_{\min}}^{\infty} J_{\text{rel}}(p) dp}{X_{\text{rel}}(\omega, \theta, p_{\min}) J_{\text{rel}}(p_{\min})} = \frac{\Delta_{2\text{NR}}^2(p_{\min}) T(\omega, \theta, p_{\min})}{X_{\text{rel}}^2(\omega, \theta, p_{\min})} = \Delta_{2\text{NR}}
\]

Explicit expressions for \(\Delta_{2\text{NR}}^1\) and \(\Delta_{2\text{NR}}^2\) are
\[
\eta_{\Delta_{2\text{NR}}^1} = \frac{\eta_{\Delta_{2\text{NR}}^2}}{n_\text{DDCS}_{\text{NR}}}
\]
where \(\eta_{\Delta_{2\text{NR}}^1}\) is expressed in terms of \(\eta_{\Delta_{2\text{NR}}^2}\)
\[
\eta_{\Delta_{2\text{NR}}^1} = \frac{\eta_{\Delta_{2\text{NR}}^2} E^2(p_{\min}) T(p_{\min}, \omega', \theta)}{X_{\text{rel}}^2(p_{\min}, \omega', \theta)}
\]
The \(S_{\eta}\) factor for the K-shell is given as
\[
S_{10} = 1/4
\]
and the \(S_{\eta}\) factor for the L subshells is given as
\[
S_{20} = \frac{p_{\min}^2}{3} + \frac{(\alpha Z m)^2}{480}
\]
\[
S_{21} = \frac{p_{\min}^2}{3} + \frac{(\alpha Z m)^2}{160}
\]

See appendix E for the M and N shell \(S_{\eta}\) factors and the mathematical details for how these above equations were derived.

2.5. Comparisons of the accuracy of various expressions for the K-shell \(\Delta_2\)

Values for the exact relativistic expression for the K-shell \(\Delta_2\), which is obtained by the numerical integration of \(I_2\)
(25) and DDCS (8), using equations (A1)–(A3) to calculate \(\rho_{\text{rel}}\) (11) (num in figure 1), is compared to \(\eta_{\Delta_{2\text{NR}}^2}\)
(NR in figure 1), derived from NR Coulombic wavefunctions but with relativistic kinematics (see equations (39) and (41)). Further comparisons are drawn to the low Z limit of \(\eta_{\Delta_{2\text{NR}}^2}\) (NR-LZ in figure 1), which is also based on equations (39) and (41) but with \(E(p_{\min})\) replaced by \(m\). This is represented by \(\eta_{\Delta_{2\text{NR}}^2}\). In addition, comparisons are drawn to the fully relativistic factored out \(X_{\text{rel}}\) (see equation (F1)), \(\eta_{\Delta_{2\text{NR}}^2}\) (rel in figure 1). All versions of \(\Delta_2\) are plotted as functions of \(p_{\min}\) in the atomic units. In both the high and low Z cases, \(\eta_{\Delta_{2\text{NR}}^2}\) and \(\eta_{\Delta_{2\text{NR}}^2}\) provide the best agreement with numerical \(\Delta_{2\text{NR}}\) slightly more accurate around \(p_{\min} = 0\); however, it is slightly less accurate at large \(p_{\min}\). The latter result is probably attributed to the infinite series in equation (D1) being carried only up to \(p_{\min}^2\). The expansion of equation (D1) to terms beyond \(p_{\min}^2\) should improve the accuracy for a very large \(p_{\min}\). \(\eta_{\Delta_{2\text{NR}}^2}\) is reasonably accurate when \(p_{\min}\) is small; however, it rapidly diverges with increasing \(p_{\min}\). This result demonstrates why the Ribberfors’ assumption of \(E \approx m\) is fatal.

2.6. Requirements for the successful extraction of a Compton profile from a DDCS spectrum

The most essential requirement for obtaining an accurate CP is that the IA must itself be valid. The accepted requirement for predicting this is
\[
\frac{p_{av}}{|k|} < 1
\]
where \(p_{av} = \langle p_x^2 \rangle + \langle p_y^2 \rangle + p_{\min}^2 / 2\) represents the average momentum of the bound electron. Here, \(\langle p_x^2 \rangle = \langle p_y^2 \rangle = (\alpha Z m)^2 / 3\). Replacing \(\langle p_x^2 \rangle\) with \(p_{\min}^2 / |k|\) a more dependable predictor when IA is valid over the full \(p_{\min}\) range of a CP; see [15]. This requirement is based on the assumption of a hydrogen-like atom.

A further requirement that pertains to the RKJ expression is that its correction, if based on NR wavefunctions, must have the relativistic and factorization effects that largely cancel in \(\Delta_1\) and \(\Delta_2\). This
assumption was tested for a uranium K shell. The relativistic effects are very large, and the CP is very broad. Clearly, both relativistic effects and the loss of accuracy caused by the factorization of the kinematic factors $E$, $X_{rel}$, and $\frac{dX_{rel}}{dp}$, largely cancel each other. In figure 2, the RKJ error ranges from 25% to approximately 30%. The resulting CP when obtained using the corrected RKJ expression is well within 1% of the Biggs CP values. The NR CP has a greater magnitude at $p_{min}$; it is sharper and attenuates faster than the relativistic CP with an increase in $p_{min}$. The small component wavefunction contributes to the broadening and increased amplitude of the extremes of the CP, see figures and discussion in appendix D for a uranium K-shell example of this behavior.

The screening effects in $\Delta_1$ and $\Delta_2$ also largely cancel each other. In figure 3, the RKJ error is approximately 6% for the $3d_{3/2}$ CP of uranium. The error is reduced to approximately 1% after the RKJ expression is corrected. The magnitude of the NR coulombic CP is considerably smaller around $p_{min}$; it has a greater magnitude at the extremes. This figure demonstrates how well the screening factors cancel the RKJ correction expressions.

3. Systematic analysis of the limitations of the rkj expression

The contributions of $KJ/E$, $CI_1$, and $CI_2$ in the integrated by parts RIA expression for the DDCS in equation (23) are illustrated in figure 4. In figure 4(a), $Z = 92$ with $\theta = 180^\circ$ was selected because the contributions of $CI_1$ and $CI_2$ to DDCS are maximized. Here, the RKJ approximation yields a DDCS Compton peak, whose maximum magnitude is approximately 43% greater than that of the RIA peak. The expected error is virtually zero if one assumes $E \approx m$, along with $CI_2 \ll K_{red}/E$, which was done previously by Ribberfors [1].

The peak magnitude decreases compared to the uncorrected RKJ expression when $CI_1$ is combined with $K_{red}/E$. The full RIA Compton peak is obtained when $CI_2$ is added to $C(JX/E + I_1)$, as expected. The contribution of $I_2$, although smaller than $I_1$, is by no means negligible. Although the magnitudes of RIA and RKJ
Compton peaks are very different, the positions of their maxima on the $\omega$ scale are similar. The magnitudes of the correction integrals $I_1$ and $I_2$ decrease more slowly than those of the DDCS as one moves away from the peak maximum on either side. This indicates that the relative size of the RKJ error becomes progressively larger as one approaches the extremities.

In figure 4(b), the same calculation is performed, but with $\theta = 90^\circ$. Here, the error in the RKJ approximation is considerably smaller than that when $\theta = 180^\circ$. This is because $I_1$ becomes positive, which partially cancels the negative $I_2$. The relative contribution of $I_2$ to the DDCS is the same as that when $\theta = 180^\circ$.

$\omega$, $Z$, and $\theta$ in figure 4(c), are the same as that in figure 4(b); however, the calculation of $I_1$ is performed by replacing $E(p)$ with $m$ when deriving the expression for $dX^{rel}/dp$. $I_2$ was assumed to be negligible, as also considered by Ribberfors to obtain equation (53) in [1]. In this example, $I_1$ corrects the RKJ approximation in the wrong manner when $\theta = 90^\circ$. Here, the resulting Compton peak magnitude is too large. Further, according to equation (52) in [1], $dX^{rel}/dp$; therefore, $I_1$ goes to 0, as $\theta \rightarrow 180^\circ$. This derivative has its maximum value when $\theta = 180^\circ$, see figure 6 and equation (26), which was derived with no assumptions.
3.1. Z dependence of $\Delta_1$ and $\Delta_2$

Calculated results for the Z dependence of the K-shell $\Delta_n$, $\Delta_1$, and $\Delta_2$ are shown in figures 5(a) and (b), where $\omega_1 = 662$ keV with $\theta = 180^\circ$ and $90^\circ$, respectively. Here, $\Delta_1$, $\Delta_2$, and $\Delta_3 = \Delta_1 + \Delta_2$ are obtained at the respective peak maxima for I$_1$, I$_2$, and DDCS. When $\theta = 180^\circ$ (figure 5(a)), both $\Delta_1$ and $\Delta_2$ are negative and vary roughly in proportion to $Z^2$, even if $Z$ is high. When $\theta = 90^\circ$ (figure 5(b)), $\Delta_1$ is now positive and varies monotonically in proportion to the power of $Z$ between one and two, but it is closer to two, whereas $\Delta_2$ is unchanged from the $\theta = 180^\circ$ results. In both cases, $\Delta_3 \rightarrow 0$ as $Z \rightarrow 0$.

3.2. $\theta$ dependence of $\Delta_1$ and $\Delta_2$ and the $\theta \rightarrow 0^\circ$ limits of $X^{rel}$ and $dX^{rel}/dp$

We investigate the dependence of $\Delta_1$, $\Delta_2$, and $\Delta_3$ on $\theta$; $\Delta_1$ is strongly dependent on $\theta$ and it approaches zero as $\theta \rightarrow 0^\circ$, whereas $\Delta_2$ is independent of $\theta$. As $\theta \rightarrow 0^\circ$, $X^{rel}$ approaches its NR limit $X^{NR} = 1 + \cos^2 \theta$, while becoming independent of $p$ and $\omega$. The resulting $X^{NR}$ can factor out integrals in $\Delta_2$. This and the fact that $\Delta_1 \rightarrow 0$ as $\theta \rightarrow 0^\circ$ are used to obtain a very simple expression to correct the RKJ formula.

The results illustrated in figure 6 reveal that $\Delta_1$ is strongly $\theta$-dependent and its maximum value occurs when $\theta = 180^\circ$. The position of the sign change for $\Delta_1$ is dependent on $\omega$. In section 3.3, it is demonstrated that the position of this sign change of $\Delta_1$ approaches $\theta = 90^\circ$ because $\omega_1 \rightarrow \infty$. Further, $\Delta_2$ is independent of $\theta$ (also $\omega$).

It can be proven that $\Delta_1 \rightarrow 0$ results as $\theta \rightarrow 0^\circ$. The $\theta$ dependence of $\Delta_1$ is attributed to the presence of $dX^{rel}/dp$ in the integrand of I$_1$. As $\theta \rightarrow 0^\circ$, $A \rightarrow 0$ (see equation (27)) and $B \rightarrow 0$ (equation (28)) provided $|\hat{K}| = 0$. The result is that $dX^{rel}/dp \rightarrow 0$. If $|\hat{K}| = 0$, as $\theta \rightarrow 0^\circ$, one can employ the LH $\delta$ pits rule. The result is that $A/|\hat{K}|^2 \rightarrow 1$ and $B \rightarrow 1$, and all other terms in $dX^{rel}/dp$ go to zero except for $\pm 2/\omega_1^2$, both of which cancel again, yielding $dX^{rel}/dp \rightarrow 0$ as $\theta \rightarrow 0^\circ$.

As $\theta \rightarrow 0^\circ$, $X^{rel}$ can be factored out of both the numerator and denominator of $\Delta_2$, which can then cancel out. However, if $Z$ is nonzero, $\Delta_2$ remains nonzero (see figure 6). In principle, $\Delta_2$ would be zero if one assumes...
$E = m$ before integrating equation (8) by parts. Thus, $I_2$ must not be disregarded, especially when $E_b$ is large. The $\theta \to 0$ limit of $I_2$ and the DDCS are

$$
\lim_{\theta \to 0^+} I_2 = \lim_{\theta \to 0^+} \int_{p_{\text{min}}}^{\infty} \frac{I_{\text{rel}}(p) X^{\text{rel}}(\omega, \theta, p) dp}{E(p)} \approx X^{\text{NR}}(\theta) \int_{p_{\text{min}}}^{\infty} \frac{p I_{\text{rel}}(p)}{E(p)} dp
$$

$$
\lim_{\theta \to 0^+} \text{DDCS} = \lim_{\theta \to 0^+} C \int_{p_{\text{min}}}^{\infty} \frac{p I_{\text{rel}}(p) X^{\text{rel}}(\omega, \theta, p) dp}{E(p)} \approx C X^{\text{NR}}(\theta) \int_{p_{\text{min}}}^{\infty} \frac{p I_{\text{rel}}(p)}{E(p)} dp
$$

Such results can be used to correct the RKJ expression in the small $\theta$ regime. The resulting simplified expression to correct the RKJ expression in the limit of low $\theta$ after $E(p)$ is factored outside the integrals with the assumption that $\Delta_1 \approx 0$, is valid when $\theta < 50^\circ$ (see figure 6) and is given by

$$
J(p_{\text{min}}) = \frac{[1 - \Delta_1(p_{\text{min}})] \text{DDCS}(\omega, \theta, p_{\text{min}})}{C(1 + \cos^2 \theta)}
$$

$\Delta_2$ appears to represent the magnitude of the relative difference between the RIA expressions in which $E(p)$ is under the integral of equation (8) and the same expression with $m$ in place of $E(p)$, now outside the integral. This factor is defined as

$$
\Delta_{em} = \int_{p_{\text{min}}}^{\infty} \frac{p I_{\text{rel}}(p) dp}{E(p)} - \frac{1}{m} \int_{p_{\text{min}}}^{\infty} \frac{p I_{\text{rel}}(p) dp}{E(p)}
$$

where $(1/m) \int_{p_{\text{real}}}^{\infty} p I_{\text{rel}}(p) dp = (1/m) I_{\text{rel}}(p_{\text{max}})$ is used. The evidence for this is that $\Delta_2$ and $\Delta_{em}$ appear to be numerically equivalent; this apparent equivalence is demonstrated to exist over a broad range of $\theta, \omega_i$ and $Z$ by comparisons between $\Delta_2$ and $\Delta_{em}$ in figures 6 and 8.

---

**Figure 5.** Dependence of K-shell $\Delta_1, \Delta_2$ and $\Delta_t = \Delta_1 + \Delta_2$ on Z. $\Delta_1 = CI/\text{DDCS}$ and $\Delta_2 = CI/\text{DDCS}$. All values are obtained by taking the maximum amplitudes for $I_1, I_2$, and DDCS using equations (24), (25) and (8) respectively. $\omega_i = 662$ keV, figure 5(a) $\theta = 180^\circ$, and figure 5(b) $\theta = 90^\circ$. 
3.3 Dependence of $\Delta_1$ and $\Delta_2$ on $\omega_i$ and the $\omega_i \to \infty$ limit of $X^{rel}$ and $dX^{rel}/dp$

The $\omega_i \to \infty$ limit of $\Delta_1$ is $I_1/DCS$ at a fixed $\theta$ is considered. It is assumed that the value of $\omega_f$ at which the CP $J$ is at its maximum value—around where $p_{min}^0 = \omega_f$—approaches a finite constant as $\omega_i \to \infty$ to ensure that this limit is valid around the Compton peak region. This assumption can be justified by considering the $\omega_i \to \infty$ limit of the Compton formula for scattering a free stationary electron at a given $\omega_i$ and $\theta$. This Compton formula can be derived from the expression for $p_{min}^0$ by setting $p_{min}^0 = \omega_f$ and solving for $\omega_f$. Here, $w_{pk}$ corresponds to the position of the Compton line.

Thus, the following limit arises.

$$\lim_{\omega_i \to \infty} \omega_f^{pk} = \lim_{\omega_i \to \infty} \frac{m\omega_j}{m + \omega_i(1 - \cos \theta)} = \frac{m}{1 - \cos \theta}.$$  \hfill (49)

The above equation demonstrates that $\omega_f^{pk}$ remains finite unless $\theta$ is exactly zero because $\omega_i \to \infty$. As a result, $F \to W = \omega_f(1 - \cos \theta)$ (Equation (13)) and $|\vec{K}| \to \omega_f$ as $H \to 0$ (Equation (18)); then, $\lim_{\omega_i \to \infty} V^{1/2} = W(E(p) + \omega_i \cos \theta)/\omega_f$ (Equation (16)) and $\lim_{\omega_i \to \infty} V^{1/2} = W$ (equation (17)). The terms starting with $m^2/\omega_f^2$ in equation (12) and those starting with $m^2/\omega_f^2$ in equation (26) go to zero or to a constant (with respect to $\omega_i$). The following equations are obtained using such limits, along with the assumption that $\theta > 0^\circ$.

$$X^{rel}_{hi}(\omega_i, \theta, p) = \lim_{\omega_i \to \infty} \frac{\omega_i}{E(p) + \omega_f \cos \theta} + \frac{\sum_{j=0}^{\infty} \chi_j(\omega_j, \theta, E(p))}{\omega_f^2}. \hfill (50)$$

Here the symbolic $\chi_j$ terms can be disregarded because, as $\omega_i \to \infty$, the first term approaches $\infty$, whereas the terms represented by $\chi_0$ approach a finite limit and a higher $j$, and terms represented by $\chi_j$ approach zero, which result in

**Figure 6.** Dependence of K-shell $\Delta_1$, $\Delta_2$, $\Delta_t = \Delta_1 + \Delta_2$ and $\Delta_{em}$ for $\theta$. The labels and formulas are the same as those in figure 5. $\Delta_{em}$ is defined by (48), $\omega_i = 662$ keV; figure 6(a), $Z = 92$; figure 6(b), $Z = 62$; and figure 6(c), $Z = 29$. 

Figure 7. High $\omega_i$ limit of $T(\omega_i, \theta, 0)/X_{\text{rel}}(\omega_i, \theta, 0)$. Dependence of $T(\omega_i, \theta, 0)/X_{\text{rel}}(\omega_i, \theta, 0)$ on $\omega_i$ and $\theta$ at $p_{\text{min}}=0$. Values obtained using equations (12) and (26). The labels hElm for the $\omega_i \to \infty$ limit, obtained from $T_{hE}^{\omega_i}(\omega_i, \theta, 0)$ (see equation (52)), and the remaining six curves are labeled according to $\omega_i$ in keV.

$T_{hE}^{\omega_i}(\omega_i, \theta, p) = \lim_{\omega_i \to \infty} T(\omega_i, \theta, p) = \omega_i \left[ \frac{\omega^2 f_i^2 \sin^2 \theta}{W^2 [E(p) + \omega_f \cos \theta]^2} - \frac{1}{E(p) [E(p) + \omega_f \cos \theta]^2} \right] + \sum_{k=0}^{4} \frac{\tau_k(\omega_i, \theta, E(p))}{\omega_i^4},$ (51)

where the $\tau_k$ terms can be disregarded. Thus, if the $\chi_j$ and $\tau_k$ terms are disregarded, the ratio of equations (51) to (50) is

$\frac{T_{hE}^{\omega_i}(\omega_i, \theta, p)}{X_{\text{rel}}^{\omega_i}(\omega_i, \theta, p)} = \lim_{\omega_i \to \infty} \frac{T(\omega_i, \theta, p)}{X_{\text{rel}}(\omega_i, \theta, p)} = \left( \frac{\omega f_i \sin \theta}{W [E(p) + \omega_f \cos \theta]} \right)^2 - \frac{1}{E(p) [E(p) + \omega_f \cos \theta]}.$ (52)

The above equations are used to obtain the following expression for $\Delta_1$:

$\Delta_1(\omega_i, \theta, p_{\text{min}}) = \frac{\omega f_i}{m \omega_i^2}(p_{\text{min}})^2E^2(p_{\text{min}})^2 \left[ \frac{\omega f_i \sin \theta}{W [E(p_{\text{min}}) + \omega_f \cos \theta]} \right]^2 - \frac{1}{E(p_{\text{min}}) [E(p_{\text{min}}) + \omega_f \cos \theta]}.$ (53)

This equation is derived by substituting equations (52) into (40). In this high energy limit,

$K_{E}^{\omega_i}(p_{\text{min}}) = \frac{C\omega_i}{E(p_{\text{min}}) [E(p_{\text{min}}) + \omega_f \cos \theta]}.$ (54)

is obtained by substituting the first term in equations (50) into (20). Then, equations (53) and (54) along with (39) can be substituted into equation (32) to obtain a corrected RKJ expression valid at high energy.

A different approach reported by Florescu and Pratt [27] were used to obtain the high-energy limit of $X_{\text{rel}}^{\omega_i}$. They assume that the ratio $\eta = \omega_f/\omega_1 > 0$, while $\theta = 0^\circ$ as $\omega_i \to \infty$. Here, $\theta$ is a function of $\omega_i$, i.e., $\theta(\omega_i)$. Their result given by equation (79) in [27] is independent of $\theta$ and corresponds to the same limit that one would obtain by assuming that the photon scattering is off of a stationary free electron. Their expression is consistent with the equation (50) when $p_{\text{min}}=0$ or when $\omega_f = \omega_f^{\text{min}}$; however, it is not over the rest of the Compton $p_{\text{min}}$ spectrum. The present limit works well for correcting the RKJ at any fixed $\theta$.

In the special case, where $p_{\text{min}}=0$, the assumption considered when performing calculations illustrated in figures 4–8 by taking the peak maximum values for $I_1$, $I_2$, and DDCS, and the above three equations (50)–(52) is reduced to

$X_{hE}^{\omega_i}(\omega_i, \theta) = \lim_{\omega_i \to \infty} X_{\text{rel}}^{\omega_i}(\omega_i, \theta) = \lim_{\omega_i \to \infty} \frac{m}{m - W} = \frac{\omega_i}{m} (1 - \cos \theta),$ (55)
Figure 7 shows that the ratio \( T(\omega, \theta) / X^{\text{rel}}(\omega, \theta) \) from equations (12) and (26) with \( p_{\text{min}} = 0 \) approaches a constant as \( \omega_i \) increases above 5 MeV. This limit is valid over \( \theta \) and is in excellent agreement with the high \( \omega_i \) limit predicted by equation (57). Equation (56) demonstrates that \( T_{\text{HE}}(\omega, \theta) \) is 0 when \( \theta = 0^\circ \) and when \( \theta = 90^\circ \). The results shown in figure 7 confirm both predictions and the high \( \omega_i \) limit of \( T_{\text{HE}} / X^{\text{rel}} \). When \( \theta = 90^\circ \), A and B containing terms in equation (56) exactly cancel each other out.

In figure 8, for \( \theta = 180^\circ \), \( \Delta_1 \) has the most negative value; at 80\(^\circ\), \( \Delta_1 \) is positive. In all cases, \( \Delta_1 \), which is obtained from the maximum values for \( I_1 \) and DDCS (with respect to the \( \omega_i \) scale), reaches a constant value as \( \omega_i \) increases above approximately 10 MeV, whereas \( \Delta_2 \), which is obtained at the peak maximum, is independent of both \( \omega_i \) and \( \theta \). Figure 8(d) shows that it is possible for \( \Delta_1 \) to change the sign. The results in figure 6 confirm that \( \Delta_{\text{em}} \approx \Delta_2 \) overall \( \omega_i \) and \( \theta \). This demonstrates that \( \Delta_2 \) is independent of these two variables, but it is approximately proportional to \( Z^2 \) or \( E_F \) for any given subshell.

4. Validity of corrected RKJ expressions for CP obtained from RIA DDCS

We demonstrate that it is possible to obtain an accurate CP from DDCS, even when the RKJ expression breaks down. For test calculations, the DDCS is computed from screened relativistic wavefunctions. These DDCSs were obtained by the numerical integration of equation (8) using the Dirac–Fock–Slater potential of Cromer and Waber [28]. The validity of the analytic expressions for correcting the RKJ approximation is put to the test by comparing CP obtained from these RIA DDCS to those obtained by the DiracHartree–Fock calculations of Biggs et al [26].

All calculations of CP obtained from DDCS exclude non-RIA features such as the infrared rise (or divergence) and resonances [15, 16]. Further, this is true for the CP from Biggs [26], which is based on the Fourier transformed electron wavefunctions (not involving IA). In almost all cases, a widely accepted
requirement to extract a CP from a full DDCS spectrum successfully, i.e., $p_{\text{corr}}/|\vec{k}| < 1$, was met. However, the results demonstrate that large errors can still occur even for a more restrictive condition $p_{\text{corr}}/|\vec{k}| \ll 1$. For most calculations in this section, $n_{\text{r}}\Delta_{\text{NR}}^2$ for $\Delta_2$ (Equation (39)) and $n_{\text{r}}\Delta_{\text{r}}^2$ (equation (40)) for $\Delta_1$ were substituted into equation (32) because it consistently provides good results (figure 1). However, $n_{\text{r}}\Delta_{\text{ef}}^2$ (equation (F1)) and $n_{\text{r}}\Delta_{\text{r}}^2$ (equation (F2)) were used for some K-shell cases, which also yielded good results.

### 4.1. Z dependence of the RKJ error

RKJ errors when obtaining $I(0)$ from RIA DDCS over a broad range of $Z$ for various subshells are summarized in Table 1. Here, $\theta = 180^\circ$, which is the scattering angle at which the RKJ error is maximized. The RKJ error for the K-shell $I(0)$ is greater than 30% for $Z = 100$, and it remains significant down to approximately $Z \approx 30$. The IA (not including the RKJ) error for the heavy atom K-shell CP at $\omega_i = 662$ keV is clearly present. This IA error is virtually eliminated when $\omega_i$ is increased to 10 MeV, whereas the remaining RKJ error is approximately 30%. This error is reduced to approximately 1% when the RKJ correction is employed.

The RKJ error for the $2s_{1/2}$ subshell of uranium is approximately one-fifth of that for the K-shell. However, the RKJ error increases to approximately 16% for the corresponding $2p_{1/2}$ subshell CP. In Table 1, the small difference between $E_{\text{rel}}$ and $E_{\text{calc}}$ for the high $Z$ K-shell CP demonstrates the degree to which relativistic factors cancel in $\Delta_1$ and $\Delta_2$ (figure 2). The results shown for the higher shell $I(0)$, where large errors are reduced to small

| nlj | Z  | $I_{\text{Biggs}}$ | $\omega_i$(MeV) | $E_{\text{ac}}$ | $E_{\text{fl}}$ | $E_{\text{rel}}$ |
|-----|----|------------------|-----------------|-------------|-------------|-------------|
| 1s_{1/2} | 100 | 0.00646 | 0.662 | 33.1 | 2.79 | 5.11 |
| 10.0 | 0.300 | 1.16 | 0.71 |
| 92 | 0.00743 | 0.662 | 29.3 | 2.81 | 4.10 |
| 10.0 | 0.261 | 0.36 | 0.67 |
| 62 | 0.0127 | 0.662 | 16.1 | 1.18 | 0.94 |
| 10.0 | 0.136 | 0.08 | 0.08 |
| 38 | 0.0221 | 0.662 | 7.33 | 0.15 | 0.36 |
| 10.0 | 0.602 | 0.45 | 0.59 |
| 29 | 0.0301 | 0.662 | 6.64 | 2.46 | 2.59 |
| 10.0 | 5.88 | 2.66 | 2.66 |
| 12 | 0.0745 | 0.662 | 2.15 | 1.41 | 1.42 |
| 10.0 | 2.01 | 1.40 | 1.40 |
| 2s_{1/2} | 92 | 0.0267 | 0.662 | 5.62 | 0.26 |
| 2p_{1/2} | 100 | 0.0111 | 0.662 | 19.2 | 4.75 |
| 2p_{3/2} | 92 | 0.1128 | 0.662 | 15.9 | 3.13 |
| 3s_{1/2} | 100 | 0.0340 | 0.662 | 13.3 | 3.03 |
| 3p_{1/2} | 62 | 0.0223 | 0.662 | 7.09 | 0.70 |
| 3p_{3/2} | 38 | 0.0406 | 0.662 | 3.30 | 0.81 |
| 3d_{5/2} | 100 | 0.0218 | 0.662 | 7.02 | 1.29 |
| 92 | 0.0243 | 0.662 | 5.99 | 1.14 |
| 79 | 0.0297 | 4.71 | 1.08 |
| 62 | 0.0412 | 3.35 | 1.07 |
| 50 | 0.0563 | 2.58 | 1.06 |
| 3d_{3/2} | 92 | 0.0252 | 0.662 | 5.95 | 0.95 |
| 4f_{5/2} | 100 | 0.0404 | 0.662 | 3.32 | 1.73 |
| 92 | 0.0472 | 3.20 | 1.23 |
| 79 | 0.0666 | 3.00 | 0.25 |
| 4f_{7/2} | 92 | 0.0479 | 3.20 | 1.23 |

Table 1. Correction of RKJ error at $p_{\text{corr}}=0$ with $\theta = 180^\circ$. $I_{\text{Biggs}}$ represents CPs from Biggs et al [26]. $E_{\text{ac}} = (|I_{\text{ac}} - I_{\text{Biggs}}|)/|I_{\text{Biggs}}| \times 100\%$, where $I_{\text{ac}}$ represents the CP obtained from the DDCS using the uncorrected RKJ formula given by equation (32) with $\Delta_1 > 0$. $E_{\text{fl}} = (|I_{\text{fl}} - I_{\text{Biggs}}|)/|I_{\text{Biggs}}| \times 100\%$ is the corrected RKJ error, where $I_{\text{fl}}$ denotes the full RKJ correction obtained from equation (33) using (40) for $\Delta_1$, and equation (39) for $\Delta_2$. $E_{\text{rel}} = (|I_{\text{ac}} - I_{\text{Biggs}}|)/|I_{\text{Biggs}}| \times 100\%$, where $I_{\text{ac}}$ is obtained from equation (32) using equation (F.83) for $\Delta_1$ and equation (F.84) for $\Delta_2$.
ones using such RKJ correction factors, appear to demonstrate a large cancelation of screening effects (figure 3). The requirement \(|p_k/\bar{k}| < 1\) was easily met for all results listed in table 1.

The strong j quantum number dependence of the RKJ error is also illustrated here. Examples are provided for the L-shell CP and continued to the M-shell CP and beyond. The RKJ error is significant even for the 4f subshell; however, it becomes negligible for 4d, 4p, 4s, and for higher shell CPs. There are significant differences in the RKJ errors for pairs of j states. For example, the RKJ error for uranium 2p_{1/2} is −15.9% while it is only −12.1% for 2p_{3/2}. For the RKJ error remaining after it is corrected, \(E_j\) illustrates some under-correction for the former and over-correction for the latter. If the error for the corrected 2p_{1/2} and 2p_{3/2} correspond to electron populations, the net remaining error is greatly reduced as in an entire-atom CP. The difference in the corrected j (spin orbit) state CP error values decrease with increasing n (primary quantum number). One would need to use a correction based on Dirac wavefunctions, similar to the K-shell expressions given in appendices D and F, to achieve greater accuracy with respect to j.

4.2. Comparison of how well the performances of the three kinematic versions for the RKJ correction work for the K and L shell CPs

The validities of the three kinematic versions of the RKJ correction are shown in figures 9 and 10 and summarized in tables 2 through 9. Here, an accuracy of within a few percent error over 99% of the electron momentum distribution range for the CP is achieved when full kinematic expressions are used to correct the RKJ. The small angle expression, which is based on equation (47), shows poor results at \(\theta = 180^\circ\) (see figures 9(a), (b), 10(a) and (b); also see tables 2 and 3). At 662 keV, this small-angle RKJ expression yields good results for \(\theta < \) less than approximately 30°.

The high energy limit RKJ correction yields poor results at \(\omega_1 = 662\) keV (see figures 9(a), (c), 10(a), and (c)), but it yields good results at 10 MeV (figures 9(b), (d), 10(b) and (d); tables and 9). At \(\theta = 30^\circ\), the small-angle RKJ correction works well when \(\omega_1 = 662\) keV, but not when \(\omega_1 = 10\) MeV. This is because one must progressively decrease \(\theta\) to be in a NR regime with an increase in the energy (equation (25) in [20]). Good results

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**Figure 9.** Correction of RKJ error for Uranium K-shell CP using four versions of the kinematic factors. Labels: Biggs for CP from tables of Biggs [26], Full K for CP obtained by using equation (32), where \(\Delta_1\) is replaced with \(\omega_1 \Delta_0^{NR}\), using equation (40) along with \(S_{\omega_1}\) using equation (41). Here \(\Delta_1\) is replaced by \(\omega_1 \Delta_0^{NR}\) using equation (39). Uncor for uncorrected RKJ expression obtained by using equation (32) with \(\Delta_1 = \Delta_0 = 0, \theta \to 0^\circ\) for small angle approximation using equation (47), \(\theta \to 0^\circ\) for small angle limit with relativistic K CP obtained from equation (47) with \(1 + \cos\theta\) replaced by \(K_{\omega_1}\) equation (20), HE lim for high energy limit where CP is obtained by using equation (32) with \(\Delta_1\) replaced by \(\omega_1 \Delta_0^{NR}\) see equation (53) and \(\Delta_0\) replaced by \(\omega_1 \Delta_0^{NR}\).
are obtained for the small $\theta$ approximation when $\theta = 5^\circ$ at 10MeV. Figure 9(d) shows that replacing $K_{NR}$ with $K_{rel}$ significantly improves the small-angle RKJ corrections when $\theta = 30^\circ$. Similar results are obtained for the subshell. See figure 10 for $2p_{1/2}$, and tables 2–9.

The requirement $p_{min}/|\vec{k}| < 1$ is easily met for all but one result in tables 1–10. The exception is in table 2, where $\omega_1 = 662$ keV and $\theta = 5^\circ$; here, $p_{min}/|\vec{k}| \approx 10$. When $\omega_1$ is increased to 10MeV (see table 3), the IA requirement is met with a $p_{min}/|\vec{k}| \approx 0.5$.

The RKJ error is considerably smaller at $\theta$ less than approximately 90°, which is partly because the $\Delta_1$ and $\Delta_2$ components of the RKJ error partially cancel at scattering angles of approximately between 60° and 90°. Interestingly, when $K_{NR}$ is replaced by $K_{rel}$, this small $\theta$ correction works fairly well at $\theta$ as large as 120°. This is

![Figure 10. Same labels as those in figure 9 but for Uranium $2p_{1/2}$ CP. See equation (43) for the $S_{21}$ factors.](image)

| $\theta$ (deg) | $p_{min}$ | $J_{Biggs}$ | $Q$ | $E_{sc}$ | $E_{ft}$ | $E_{rel}$ | $E_{SAK}$ | $E_{HE}$ |
|---------------|-----------|-------------|-----|---------|---------|-----------|-----------|---------|
| 180           | 0         | 0.00743     | 1.0 | −29.3   | 2.83    | 4.13      | 52.1      | −21.4   | 73.6    |
|               | 60        | 0.0033      | 0.444 | −30.9 | 4.55    | 5.21      | 20.2      | −21.5   | −88.5   |
|               | 100       | 0.0013      | 0.175 | −33.8 | 6.50    | 6.43      | 5.53      | −23.2   | 106.0   |
| 120           | 0         | 0.00743     | 1.0 | −16.3   | −3.16   | −2.62     | 88.8      | −6.86   | 52.6    |
|               | 60        | 0.0033      | 0.444 | −17.9 | −1.99   | −1.61     | 69.1      | −6.82   | 70.9    |
|               | 100       | 0.0013      | 0.175 | −20.4 | −2.18   | −2.22     | 61.3      | −7.67   | 95.6    |
| 60            | 0         | 0.00743     | 1.0 | −8.73   | −2.42   | −2.06     | 22.2      | 1.64    | 50.2    |
|               | 60        | 0.0033      | 0.444 | −4.34 | −2.93   | −3.40     | 15.7      | 2.55    | 30.9    |
|               | 100       | 0.0013      | 0.175 | −1.83 | −1.56   | −1.56     | 13.6      | 1.62    | 28.4    |
| 5°            | 0         | 0.00743     | 1.0 | −13.9   | −1.75   | −1.21     | −1.75     | −1.75   | 410.9   |
|               | 60        | 0.0033      | 0.444 | −10.8 | 0.70    | 0.99      | 0.65      | 0.61    | 555.0   |
|               | 100       | 0.0013      | 0.175 | −11.2 | 3.01    | 3.09      | 2.64      | 2.29    | 6408    |

Note.

* From the relativistic Coulombic DDCS.
because most errors in the small angle expression at small to moderate $\theta$ are present in the NR kinematic factor $X_{NR}$. In addition, $\Delta_1$ is close to zero at a small to moderate $\theta$ (figure 6).

The high-energy correction of RKJ does not work very well when $\omega_i = \Delta 662$ keV; however, it is considerably good at 10 MeV. Here, energies in the MeV regime are required for such expressions to be valid (figures 7 and 8). Further, this correction method breaks down at a very small angle ($\theta = 5^\circ$). Even at energies as high as 10 MeV, one must go to an even higher $\omega_i$ for obtaining accurate values for $J$ (see assumptions made when deriving

| $\theta$ (deg) | $p_{min}$ | $J_{Bigg}$ | $Q$ | $E_{sw}$ | $E_{fl}$ | $E_{SA}$ | $E_{SAK}$ | $E_{HE}$ |
|---------------|-----------|------------|-----|---------|---------|---------|-----------|---------|
| 180           | 0         | 0.0743     | 1.0 | -26.1   | -0.36   | 0.67    | 65.9      | -17.8   | 3.50    |
| 60            | 0.0033    | 0.444      | -25.6| 0.13    | 0.75    | 12.4    | 15.6      | 4.14    |
| 100           | 0.0013    | 0.175      | -27.5| 0.67    | 0.61    | -12.0   | -15.9     | 5.00    |
| 120           | 0         | 0.0743     | 1.0 | -18.8   | -2.83   | -2.21   | 114.5     | -9.69   | -0.27   |
| 60            | 0.0033    | 0.444      | -20.2| -1.10   | -1.19   | 65.6    | -9.50     | 1.47    |
| 100           | 0.0013    | 0.175      | -22.6| -0.164  | -1.23   | 36.2    | -0.15     | 2.94    |
| 60            | 0         | 0.00743    | 1.0 | -10.36  | -2.69   | -2.29   | 711.6     | -0.27   | -4.58   |
| 60            | 0.0033    | 0.444      | -8.43| 2.93    | 3.20    | 618.2   | -1.61     | 4.38    |
| 100           | 0.0013    | 0.175      | -7.17| -3.51   | -3.08   | 533.1   | -3.85     | 3.51    |

Note.  
* From the relativistic Coulombic DDCS.

| $\theta$ (deg) | $p_{min}$ | $J_{Bigg}$ | $Q$ | $E_{sw}$ | $E_{fl}$ | $E_{SA}$ | $E_{SAK}$ | $E_{HE}$ |
|---------------|-----------|------------|-----|---------|---------|---------|-----------|---------|
| 180           | 0         | 0.0267     | 1.0 | -5.62   | -0.637  | -4.31   | -4.31     | -4.31   |
| 15            | 0.0142    | 0.524      | -6.43| 1.43    | 1.43    | 1.43    | 1.43      | 1.43    |
| 100           | 0.00033   | 0.0124     | -33.0| 0.606   | 0.606   | 0.606   | 0.606     | 0.606   |
| 60            | 0         | 0.0267     | 1.0 | -1.87   | -1.01   | 19.85   | 0.712     | 0.712   |
| 15            | 0.142     | 0.524      | -1.64| -0.64   | -0.64   | 23.57   | -4.93     | -4.93   |
| 40            | 0.0008    | 0.0333     | -11.6| 0.337   | 0.337   | 33.7    | 0.341     | 0.341   |

| $\theta$ (deg) | $p_{min}$ | $J_{Bigg}$ | $Q$ | $E_{sw}$ | $E_{fl}$ | $E_{SA}$ | $E_{SAK}$ | $E_{HE}$ |
|---------------|-----------|------------|-----|---------|---------|---------|-----------|---------|
| 180           | 0         | 0.0267     | 1.0 | -4.87   | -0.637  | -4.31   | -4.31     | -4.31   |
| 15            | 0.0142    | 0.524      | 15.4| 0.50    | 0.50    | 0.50    | 0.50      | 0.50    |
| 100           | 0.00033   | 0.0124     | -26.0| -3.03   | -3.03   | 1.51    | 1.51      | 1.51    |
| 90            | 0         | 0.0267     | 1.0 | -2.4    | -1.05   | -1.01   | -0.787    | -0.787  |
| 15            | 0.142     | 0.524      | -2.86| -0.643  | -0.643  | -0.571  | -0.714    | -0.714  |
| 100           | 0.00033   | 0.0124     | -10.6| -1.33   | 0.182   | 0.182   | 1.21      | 1.21    |

| $\theta$ (deg) | $p_{min}$ | $J_{Bigg}$ | $Q$ | $E_{sw}$ | $E_{fl}$ | $E_{SA}$ | $E_{SAK}$ | $E_{HE}$ |
|---------------|-----------|------------|-----|---------|---------|---------|-----------|---------|
| 180           | 0         | 0.0128     | 1.0 | -15.9   | -3.13   | -3.13   | -3.13     | -3.13   |
| 40            | 0.0048    | 0.383      | -14.1| -0.21   | -0.21   | -0.21   | -0.21     | -0.21   |
| 100           | 0.00023   | 0.018      | -24.3| -3.48   | -3.48   | -3.48   | -3.48     | -3.48   |
| 60            | 0         | 0.0128     | 1.0 | -5.91   | -1.56   | 20.3    | -1.56     | -1.56   |
| 40            | 0.0049    | 0.445      | -2.25| -0.673  | 70.2    | 3.87    | 3.87      | 3.87    |
| 20            | 0.011     | 0.859      | -4.91| -1.82   | 7.27    | 1.73    | 1.73      | 1.73    |
Table 7. Uranium 2p$_{1/2}$ Compton profiles: $\omega_i = 10.0$ MeV. The labels are the same as those in the previous tables.

| $\theta$ (deg) | $p_{\min}$ | $J_{\text{Biggs}}$ | $Q$ | $E_{\text{ex}}$ | $E_{\text{fl}}$ | $E_{\text{SAK}}$ | $E_{\text{HE}}$ |
|----------------|------------|---------------------|-----|----------------|----------------|----------------|---------------|
| 180            | 0          | 0.0128              | 1.0 | −13.2         | −3.13          | 1.33           |
| 40             | 0.00048    | 0.383               | −10.8| −2.0         | 2.80           |
| 100            | 0.00023    | 0.018               | −18.7| −4.43        | 0.87           |
| 90             | 0          | 0.0128              | 1.0 | −5.47         | −1.95          | −0.612         | −1.72         |
| 40             | 0.00048    | 0.445               | −4.08| −0.735       | −0.609         | −0.816         |
| 100            | 0.00023    | 0.018               | −8.26| −2.22        | −1.30          | −0.434         |

Table 8. Uranium 2p$_{1/2}$ Compton profiles: $\omega_i = 0.662$ MeV. The labels are the same as those in the previous tables.

| $\theta$ (deg) | $p_{\min}$ | $J_{\text{Biggs}}$ | $Q$ | $E_{\text{ex}}$ | $E_{\text{fl}}$ | $E_{\text{SAK}}$ | $E_{\text{HE}}$ |
|----------------|------------|---------------------|-----|----------------|----------------|----------------|---------------|
| 180            | 0          | 0.0152              | 1.0 | −12.13        | 1.18           |
| 30             | 0.00075    | 0.497               | −10.5| 1.15         |
| 100            | 0.000075   | 0.0050              | −18.6| 3.55         |
| 60             | 0          | 0.0152              | 1.0 | −2.76         | −0.49          | 21.4           | 0.91          |
| 40             | 0.004      | 0.263               | −2.82| −0.23        | 29.6           | 0.76           |
| 100            | 0.000075   | 0.0050              | −5.00| 1.58         |

Table 9. Uranium 2p$_{3/2}$ Compton profiles: $\omega_i = 10.0$ MeV. The labels the same as those in the previous tables.

| $\theta$ (deg) | $p_{\min}$ | $J_{\text{Biggs}}$ | $Q$ | $E_{\text{ex}}$ | $E_{\text{fl}}$ | $E_{\text{SAK}}$ | $E_{\text{HE}}$ |
|----------------|------------|---------------------|-----|----------------|----------------|----------------|---------------|
| 180            | 0          | 0.0152              | 1.0 | −9.93         | 0.526          | 5.2            |
| 30             | 0.0075     | 0.497               | −8.00| 0.520        |
| 100            | 0.000075   | 0.0050              | −15.3| 1.58         |
| 60             | 0          | 0.0152              | 1.0 | −3.95         | −0.41          | −0.40          | −0.13         |
| 45             | 0          | 0.0152              | 1.0 | −3.75         | −0.37          | 6.78           | −0.13         |
| 20             | 0.012      | 0.789               | −3.32| −0.28        | 9.24           | −0.12         |

Table 10. Uranium M Shell Compton profiles: $\omega_i = 662$ keV. Labels are the same as those in the previous tables.

| $nlj$          | $\theta$ (deg) | $p_{\min}$ | $J_{\text{Biggs}}$ | $Q$ | $E_{\text{ex}}$ | $E_{\text{fl}}$ | $E_{\text{SAK}}$ | $E_{\text{HE}}$ |
|----------------|----------------|------------|---------------------|-----|----------------|----------------|----------------|---------------|
| 3p$_{1/2}$    | 180            | 0          | 0.0584              | 1.0 | −2.40         | 1.71           |
| 10.0          | 0.013         | 0.223      | −6.92               | 5.38|
| 100.0         | 0.000085     | 0.001455   | −33.6               | −1.4|
| 60             | 0            | 0.0584     | 1.0                  | −1.23| −0.582       |
| 7.0           | 0.0264       | 0.452      | −0.795              | 0.341|
| 40             | 0.00059      | 0.101      | −2.97               | −4.86|
| 3p$_{3/2}$    | 180            | 0          | 0.034               | 1.0 | −4.12         | 1.47           |
| 15             | 0.012        | 0.353      | −6.67               | 0.55|
| 60             | 0.00051      | 0.015      | −17.3               | −2.94|
| 60             | 0            | 0.034      | 1.0                  | 2.27| −0.375       |
| 15             | 0.012        | 0.353      | 3.25                | −2.25|
| 30             | 0.0013       | 0.0382     | −6.92               | −5.07|
| 3p$_{5/2}$    | 180            | 0          | 0.0379              | 1.0 | −3.42         | 2.16           |
| 60             | 0.00035      | 0.00923    | −15.9               | 0.971|
| 3d$_{3/2}$    | 180            | 0          | 0.0486              | 1.0 | −5.99         | −1.03          |
| 20             | 0.022        | 0.453      | −3.64               | −0.727|
| 60             | 0.000144     | 0.00296    | −7.64               | 1.74|
| 60             | 0            | 0.0486     | 1.0                  | −1.85| −1.03        |
| 15             | 0.034        | 0.704      | 1.06                | 1.76|
| 40             | 0.00164      | 0.0337     | 3.66                | 2.26|
| 3d$_{5/2}$    | 180            | 0          | 0.0252              | 1.0 | −5.87         | −0.952         |
| 20             | 0.011        | 0.437      | −7.89               | −4.09|
| 60             | 0.000031     | 0.00202    | −5.68               | 3.53|
One important advantage of the high-energy RKJ correction is that the accuracy of the IA improves with increasing $\omega_i$. The uranium L-shell results are summarized in tables 4 and 5 for $2s_{1/2}$, 6 and V7 for $2p_{1/2}$, and 8 and 9 for $2p_{3/2}$. There are almost no IA errors at 662 keV. The RKJ correction greatly reduces the errors to a few percent or less, even when $Q < 0.01$. The dependence of the RKJ error on both the $l$ and $j$ quantum numbers is reflected in the results.

4.3. Results for beyond L-shell CP obtained from the full kinematic RKJ correction factor

The M and N shell CP obtained from DDCS using the full kinematic corrected RKJ expression are presented in figure 11 and 10. The RKJ error is still significant, especially for $3d$ and $3p$ CP. The RKJ error tends to be larger away from the peak maximum. Here, the uncorrected errors remaining after correction at $p_{\text{min}} = 0$ with $\theta = 180^\circ$ and $\omega_i = 662$ keV are represented in these figures as $^{3d}E_{\text{err}}$ and $^{3p}E_{\text{err}}$, respectively. The RKJ error is still significant for the uranium M shell CP, whereas the $l$ quantum number dependence continues.

The magnitude of the RKJ error for uranium $4f_{5/2}$ and $4f_{7/2}$ is approximately 3%. Here, the spin orbit ($j$ state) RKJ error dependence is negligible, and the RKJ errors for the remaining N shell states become progressively smaller and more negligible beyond the N-shell CP. Further, there appears to be a small overcorrection for the N shell CP cases, where the screening effects are larger and may not be as well canceled by using equation (32) as it was for K through the M shell CP.

4.4. Discussion on another very recent work concerning the use of the RKJ expression

Qiao et al [29] obtained whole atoms C, Cu, Ge, and Xe CP from RIA DDCS using the RKJ formula (equation (32), [29]). This formula appears to be the same as that used for the uncorrected RKJ expression in this work (equation (19)). The errors they report are for the entire-atom CP, and such errors are considerably smaller than those arising from the inner shells of those atoms. The heaviest atom for which they obtained a CP was Xe ($Z = 54$). Qiao et al [29] stated that although they consider their numerical method to calculate DDCS via RIA theory to be exact, significant errors remain for the tail region of the entire-atom CPs. They attributed this error to the large RKJ errors arising from the inner shells of the entire-atom CP. The present RKJ correction method can dramatically reduce such errors. Further, most calculations were performed at $\theta = 120^\circ$, and the errors are considerably larger at $\theta = 180^\circ$. For an indirect comparison of the results of Qiao et al regarding entire-atom Xenon calculations with the present results, see table 1 in [29], where their reported error at $p_{\text{min}} = 20 \text{ a.u.}$ was 2.3%, and at $p_{\text{min}} = 40 \text{ a.u.}$, it was 2.6%. The errors for each subshell for Uranium CP up to $4f$ are all less about 3% even under conditions under which the RKJ error is the greatest (A heavy atom, $\theta = 180^\circ$, at $p_{\text{min}} = 100 \text{ a.u.}$).

Further, they stated that their CP was asymmetrical. The CP values obtained from the RIA theory in the present work are symmetrical. The present result is consistent with the theoretical CP, which is symmetrical by
definition. This is attributed to the fact that $J_{NR}$ (Equation (2)) and $J_{el}$ (equation (22)) are even functions. A slightly asymmetrical CP may be possible if they are obtained from QED-based theories [15, 16].

5. Application of corrected RKJ expressions to extract compton profiles from full DDCS spectra

There are three components in the full DDCS spectrum; an example of such a full DDCS spectrum is shown in figure 12. This spectrum, which is for a $2p_{1/2}$ subshell of uranium, was generated from the S-matrix code of Bergstrom et al [16]. This calculation was performed at $\omega_i = 160$ keV, with $\theta = 35^\circ$. The feature in the hard photon region is the Compton peak, and a higher $\omega_i$ is required to observe the full Compton peak. The position on the $\omega_f$ scale of the DDCS spectrum depends on the kinematic variables $\theta$ and $\omega_i$. The CP is obtained from the Compton peak by dividing the kinematic factors $K_{rel}$ or $K_{NR}$. This results in a CP that is a function of $p_{min}$ and independent of $\omega_i$, $\omega_f$, and $\theta$. $p_{min}$ is a function of these three variables and determines the location of the Compton peak on the $\omega_f$ scale; however, these variables have no influence on the CP values.

The prominent feature at 95 keV is the resonance caused by a downward electron transition from $2p_{1/2}$ to $1s_{1/2}$. Such resonances result from the energy transferred to the atom during the collision process. The resonances are not accounted for in DDCS generated from IA because the IA theory assumes an instantaneous collision between a photon and a free-moving electron. The positions of such resonances are independent of kinematics provided that $\omega_i$ is sufficiently high for such a resonance to occur.

The third feature, which is located in the soft photon region of the DDCS spectrum, is the infrared rise (or divergence); its magnitude approaches infinity as $\omega_f$ approaches zero. This feature shows some dependence on $\omega_i$ and $\theta$. In this energy regime, the Compton matrix elements are proportional to the photo effect matrix elements. The infrared divergence has its greatest presence in the K-shell DDCS spectra, and it can overlap with the Compton peak. However, a greater separation between these two features can be achieved by increasing $\omega_i$. In addition, there tends to be a greater separation between the infrared rise and the Compton peak at a large $\theta$ although the Compton peak is at its lowest $\omega_f$ when $\theta = 180^\circ$.

The S-matrix code proposed by Bergstrom et al [16] was based on external field quantum electrodynamics (QED). The calculations of the matrix elements involve a numerical evaluation of the relativistic second-order S-matrix. The theory is presented in [16], which includes the relevant formulas. A self-consistent screened Dirac–Fock–Slater atomic potential [28] with a latter tail is used as the potential. The same potential was used to generate the RIA DDCS.

In NR QED theory, the three features that include the Compton peak, resonances, and infrared divergence, can be described using three independent formulas as discussed in the introduction of [16]. However, in the relativistic version of the QED theory, such as a one-on-one correspondence between formulas and the three full DDCS spectrum features, does not exist.

**Figure 12.** Full S-Matrix DDCS spectrum for Uranium $2p_{1/2}$ with $\omega_i = 160$ keV and $\theta = 35^\circ$. 

![Full S-Matrix DDCS spectrum for Uranium 2p_{1/2} with \omega_i = 160 keV and \theta = 35°.](image-url)
5.1. Extraction of Compton profiles from some K-N shell S-matrix DDCS spectra

Almost all calculations were performed at the highest incident photon energy that the S-Matrix code could tolerate. There are many instances under which an even better agreement between the S-Matrix generated CP and established tabulated values of CP can be achieved by increasing \( \omega_i \).

In Figure 13, CPs for a Holmium K-shell obtained from S-matrix DDCS are compared to the theoretical CP of Biggs [26]. The calculation was performed at \( \omega_i = 662\text{keV} \) with \( \theta = 180^\circ \), \( \theta = 120^\circ \), and \( \theta = 45^\circ \). In all three cases, the infrared rise was subtracted from the full S-matrix DDCS spectrum using a code based on the low-energy theorem (LET) [30–32]. The corrected and uncorrected RKJ formula was used to extract the CP. A more complete separation was obtained between the Compton peak, and an infrared rise could be achieved with higher incident photon energies; however, 662keV is about the maximum energy at which the S-Matrix code functions for the Ho K-shell DDCS spectrum.

At \( \theta = 180^\circ \), the CP magnitude from the S-matrix DDCS is approximately 20\% lower than the CP of Biggs at \( p_{\text{min}} = 0 \) when the uncorrected RKJ expression is used. The error was reduced to a fraction of a percent when the corrected RKJ formula was used. These results are considerably similar for \( \theta = 120^\circ \), wherein the RKJ error is only approximately 10\%. At \( \theta = 45^\circ \), the agreement is not as good as it was at a larger scattering angle because \( p_{\text{min}}/k \) is considerably larger at this smaller scattering angle. The S-matrix CP at 180\° and 120\° is symmetrical, with a slight exception on the negative \( p_{\text{min}} \) side of the peak caused by the incomplete canceling out of the infrared divergence.

In Figure 14, a full S-Matrix DDCS spectrum was obtained for the uranium K-shell at \( \omega_i = 900\text{keV} \) near the photon energy limit for the S-Matrix code with \( \theta = 180^\circ \). It was compared to the CP generated from the RIA code. At this high energy, there is only a slight overlap between the infrared rise and the Compton peak. The addition of the infrared rise to the RIA DDCS improves the agreement between the RIA and S-Matrix DDCS. The CP is then obtained from the S-Matrix and RIA DDCSs using the corrected and uncorrected RKJ expression, respectively, and they are then compared to the CP from Biggs [26]. Clearly both the corrected CPs obtained from S-Matrix and RIA DDCS were in good agreement with CP from Biggs [26]. The S-matrix CP was symmetrical.

Even better results can be achieved at \( \omega_i > 900\text{keV} \), comparing the uranium K-shell CP obtained at \( \omega_i = 662\text{keV} \) to those obtained at \( \omega_i = 10\text{MeV} \) in tables 1–3. \( \omega_i \) should be used at least 3 MeV to obtain a negligible IA error for the U K-shell at \( \theta = 180^\circ \).
The uranium $2p_{1/2}$ DDCS was recalculated (figure 12) at $\omega_1 = 420$ keV, which is at approximately the highest energy at which the S-Matrix code will function in this case. Figure 13 shows that the infrared rise is no longer on the $\omega_2/\omega_1$ scale that starts at 50 keV, but the large resonance at 95 keV remains. There is a considerable overlap between the resonance and the Compton peak. Therefore, the agreement between the S-Matrix and Biggs CPs is very poor on the negative $p_{min}$ side, but it is considerably good on the positive $p_{min}$ tail of the CP (table 11). The CP maximum is shifted to the negative side of the $p_{min}$ scale because of the presence of resonance. The agreement between the CP extracted from the RIA DDCS with Biggs is good over the entire range of $p_{min}$. In this set of calculations, $p_{min}/|\vec{k}| < 1$.

The Compton peak is shifted to a considerably higher $\omega_1$ by decreasing $\theta$ to 50° (figure 16). Although this shift to a lower $\theta$ increases $p_{min}/|\vec{k}|$, the overlap between the resonance and Compton peaks is almost eliminated. At this angle, the RKJ error is very small; however, the inclusion of the correction improves the agreement with Biggs CP on both sides of the CP up to $p_{min} \approx 40$ (table 11). This CP is nearly symmetrical with its maximum magnitude at $p_{min} \approx 0$, with a slight shift to the $-p_{min}$ side caused by a significantly diminished overlap with the resonance. The agreement breaks down at $p_{min} = -60$ because of a slight overlap between the CP and resonance. However, the comparison differs markedly around where $p_{min} = 0$. The CP from RIA and that from Biggs are flat at the top, whereas the S-Matrix CP has a magnitude approximately 12% greater than Biggs at $p_{min} = 0$. Similar results were found for uranium $2p_{1/2}$ CP; this behavior was found to persist with considerably lighter atoms, and it can be treated with the NR theory.

The $U 2p_{1/2}$ S-Matrix CP is symmetrical with respect to the $p_{min}$ scale. Further, it is independent of kinematics, and therefore, in theory, it meets the criteria for a valid CP.

Further, the CP was extracted from uranium and strontium $2s_{1/2}$ S-Matrix DDCS. In figure 17, the U and Sr $2s_{1/2}$ peaks are shifted slightly to the positive side of the $p_{min}$ scale, whereas the CP peak maxima are approximately 7% lower in value; however, they are similar in shape to those of the Biggs CP [26]. When the corrected uranium CP is shifted by $-3.0$ a.u. on the $p_{min}$ scale, such that the peak maximum is at $p_{min} = 0$, the positive side of the uranium $2s_{1/2}$ S-Matrix CP is in good agreement with Biggs, except for the extreme tail region. Further, there is considerable deviation from Biggs on the negative $p_{min}$ tail (table 12).

Modifying $\theta$ for the U $2s_{1/2}$ CP to 90° improves the agreement with the Biggs CP on both sides. At $\theta = 90°$, the CP is shifted further away from any resonance, and the RKJ error is very small at this angle. In addition, there is no qualitative difference between the CPs at the two scattering angles and $p_{min}/|\vec{k}| < 1$ over the entire range of $p_{min}$. This provides evidence for the validity of CP.

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**Figure 14.** S-Matrix DDCS spectrum for Uranium K-shell and corresponding CP. Labels S-Matrix for DDCS from the code of Bergstrom [16], RIA from RIA using equation (8), RIA+INF for DDCS from RIA with inclusion of the infrared divergence. The infrared divergence was obtained from a code based on the low-energy theorem (see [30–32]), Biggs for Biggs CP [26], SMC for CP that were obtained from S-Matrix DDCS, using the corrected RKJ expression based on equation (32), along with equations (39)–(41), SMUC for CP obtained from S-Matrix using the uncorrected RKJ expression, RIAUC CP obtained from RIA by using the corrected RKJ expression, RIAUC COP obtained from RIA by using the uncorrected RKJ expression.
When Sr CP is shifted by -1 a.u., results for both $\theta = 180^\circ$ and $\theta = 120^\circ$ are considerably similar to those of the uranium $2p_{1/2}$ CP even though $\rho_{pkav}|\langle k \rangle|$ is greater than unity over the negative $p_{min}$ range. The RKJ error in this case is very small because of the considerably smaller binding energy of the Sr compared to U.

In Figure 18, the CP was extracted from the strontium $2p_{1/2}$ and $2p_{3/2}$ S-Matrix DDCSs. The results for both were quite similar to that of the uranium $2p_{1/2}$ CP illustrated in Figure 16, although $p_{pkav}|\langle k \rangle|$ was considerably greater than the unity for the latter CP, especially on the negative $p_{min}$ side of the CP. These peaks are shifted by approximately +0.3 a.u., and it can be attributed to an IA error or a slight overlap with a weak resonance.

Some examples of the M- and N-shell S-Matrix CPs are illustrated in Figure 19. Although $p_{pkav}|\langle k \rangle| \gg 1$, the results for Sr $3s_{1/2}$ and $3p_{1/2}$ behave in a manner similar to that of the corresponding L-shell S-matrix CP. The uranium S-Matrix $3d_{3/2}$ appears to be in good agreement with Biggs on both sides of the CP; however, there is a
structure in the middle, which may be a resonance. Further, it was not possible to avoid such resonances because of the energy limitations of the S-Matrix code. The same is true for the U S-Matrix $4f^{5/2}$ CP, which appears to be in good agreement with Biggs on either side of the peak; however, there is a structure where $p_{\text{min}}$ is near zero.

5.2. Generalizations and interpretation of S-Matrix results

Individual atomic subshell CPs can be obtained from full spectrum S-Matrix DDCS. Entire-atom CP can be obtained from measured DDCS where the energy distribution of the scattered photon is observed while individual subshell DDCS cannot be measured. For one to obtain individual subshell CP, it becomes necessary to measure TDCS as a function of ejected electron energies and angles and then integrate over the electron angles to obtain individual subshell DDCS which in turn can be transformed via the corrected RKJ formulas. See discussions in [17, 27, 33] for further details.

Table 11. Uranium $2p_{1/2}$ Compton profiles from the S-Matrix DDCS; $\omega_i = 0.420$ MeV. The labels are the same as in the previous tables. Error $E^+$ error on the positive $E^+$ and negative $p_{\text{min}}$ side of the CP.

| $\theta$(deg) | $p_{\text{min}}$ | $I_{\text{Biggs}}$ | $Q$ | $E^+_{\text{up}}$ | $E^+_{\text{down}}$ | $E_{\text{up}}$ | $E_{\text{down}}$ |
|---------------|-----------------|-------------------|-----|----------------|------------------|--------------|----------------|
| 180           | 0               | 0.0128            | 1.0 | 0.63           | 14.0             | —            | —              |
|               | 20              | 0.011             | 0.859 | -20.5       | -9.0           | —             | —              |
|               | 30              | 0.0079            | 0.617 | -20.4       | -8.1           | —             | —              |
|               | 40              | 0.0049            | 0.383 | -18.0       | -4.1           | —             | —              |
|               | 60              | 0.0017            | 0.133 | -20.0       | -1.2           | —             | —              |
| 50            | 0               | 0.0128            | 1.0 | 11.7          | 14.8           | —             | —              |
|               | 20              | 0.011             | 0.859 | -9.1        | -4.5           | -4.82        | -1.82          |
|               | 30              | 0.0079            | 0.617 | -9.75       | -7.09          | -10.9        | -8.35          |
|               | 40              | 0.0049            | 0.383 | —           | —              | -8.37        | -5.7           |
|               | 60              | 0.0017            | 0.133 | —           | —              | 17.7         | 21.2           |

Figure 17. $2s_{1/2}$ CP for Uranium and Strontium. The labels are the same as those in figures 2 and 3. Label SHIFT for CP, which are shifted by $-3$ au for U and $-1$ au for Sr.
K-shell CPs from S-Matrix DDCS were found to consistently be in good agreement with those of Biggs [26] when obtained from DDCS using the corrected RKJ formulas. This appears to be due to IA being valid for the energies and angles used to obtain those CP. Beyond K-shell, $n_{s}$, $n_{p}$, $n_{d}$, and $n_{f}$ S-Matrix CPs were found in general to be in good agreement with those of Biggs [26] in the tail region but not around where $\rho_{\text{min}}$ provided that there was no overlap between the Compton peak with the infrared divergence and/or resonances. Those differences around $\rho_{\text{min}}$ appear to be quite systematic. In the case of $n_{s}$ states where $n > 1$, the S-Matrix CP is sharp like that of Biggs [26] but the magnitude at $p_{\text{min}} = 0$ is around 7% smaller with a slight shift to the positive side of the $p_{\text{min}}$ scale. When the S-Matrix CP is shifted such that its maximum is at $p_{\text{min}} = 0$, the tail of this CP is in fairly good agreement with Biggs CP [26].

S-Matrix $n_{p}$ subshell CPs were sharp around $p_{\text{min}} \approx 0$ with a 10%–12% greater magnitude than those of Biggs [26] at $p_{\text{min}} = 0$ with the latter CP being flat at the top. Differences between $n_{d}$ and $n_{f}$ S-Matrix and Biggs [26] CP around $p_{\text{min}}$ could not be clearly determined due to the possible presence of resonances. Much greater $\omega_{i}$, which would be beyond what the S-Matrix code can tolerate, would have been required to avoid this problem.

The differences between S-Matrix and Biggs [26] CP persists down to much lighter atoms than uranium such as strontium. This result suggests that the differences at the CP maxima are not purely due to relativity. The RIA

Table 12. Uranium $2s_{1/2}$ Compton profiles from the S-Matrix DDCS: $\omega_{i} = 0.420 \text{MeV}$, the CP was shifted by $-3.2 \text{ au}$ on the $p_{\text{min}}$ scale. The labels are the same as in the previous tables. Error $E$ error on the positive $E$ negative $p_{\text{min}}$ side of the CP.

| $\theta$(deg) | $p_{\text{min}}$ | $J_{\text{Biggs}}$ | $Q$ | $E_{\text{uc}}^{+}$ | $E_{\text{uc}}^{-}$ | $E_{\text{fl}}^{+}$ | $E_{\text{fl}}^{-}$ |
|--------------|------------------|-------------------|-----|-------------------|-------------------|-------------------|-------------------|
| 180          | 0                | 0.0267            | 1.0 | 12.7              | -7.1              | —                 | —                 |
| 10           | 0.020            | 0.741             | -14.0| -5.0              | -8.5              | -2.35             |
| 15.0         | 0.013            | 0.524             | -8.7 | 0.54              | -1.4              | 6.7               |
| 20           | 0.0087           | 0.383             | -8.3 | 21.8              | 12.9              | 24.1              |
| 40           | 0.00089          | 0.033             | -55.8| -22.6             | 147.2             | 293.3             |
| 90           | 0.0128           | 1.0               | -8.2 | -2.8              | —                 | —                 |
| 10           | 0.02             | 0.749             | -7.0 | -7.0              | -3.3              | -3.3              |
| 15           | 0.014            | 0.524             | -2.8 | -2.8              | 5.2               | 5.2               |
| 20           | 0.0087           | 0.326             | 1.15 | 1.15              | 19.3              | 19.5              |
| 30           | 0.0026           | 0.0974            | 6.1  | 6.4               | 89.0              | 100.0             |
| 40           | 0.00089          | 0.033             | -19.8| -19.8             | 215.7             | 180.9             |

Figure 18. Strontium $2p_{1/2}$ and $2p_{3/2}$ CP. The labels are the same as in figure 17. The shift is 1.0 a.u.
and S-Matrix DDCS were obtained by using the same Dirac-Fock-Slater potential of Cromer and Walber [28]; thus, the potential is not the source of this discrepancy, since RIA CPs, which were obtained using the same potential, were consistently in good agreement with Biggs CP [26] after using the corrected RKJ formulas to generate them. Furthermore, electron-electron correlation factors were not included in any of the three types of CP calculations, so one can eliminate correlation as the source of the discrepancy. CP generated from S-Matrix, RIA as well as those of Biggs [26] were performed with the assumption of spherical symmetry so one can eliminate that as a source for the differences. The S-Matrix formulism is based on QED theory, while RIA theory as well as Dirac Hartree–Fock theory used by Biggs [26] are not. These results suggest that this discrepancy may be attributed to non-inclusion of dynamical QED factors in the computation of theoretical CP of Biggs.

There is some possible indirect experimental evidence for the difference between beyond the K-shell S-Matrix CP and theoretical CP obtained by using equations (2) or (22). For example, Sakurai et al [5] reported larger than expected differences between theoretical entire atom Xe CP and the corresponding Xe CP obtained from measured DDCS around where \( p_{\text{min}} \). They attributed this difference to electron correlation effects. However they also reported no such deviation for helium and only slight deviation for argon CP. The rather sharp deviation for Xe CP only around where \( p_{\text{min}} \) is consistent with the present results for uranium and strontium CP (see 16–19). However Sakurai’s result for Xe only serves as supporting but indirect evidence for the existence of beyond \( \rho(p) \) factors present in measured CPs. Other factors such as electron correlation and experimental error may play a role.

Sakurai’s result with He CP which only has an occupied K-shell is in good agreement with the present results for the K-shell CP of Ho and U (see figures 13 and 14 respectively). The agreement between S-Matrix and Biggs derived CP was found to be very good after transforming them from S-Matrix DDCS using the corrected RKJ formula. Sakurai’s results of a small deviation for Ar CP is also consistent with the present results for uranium and strontium CP (see 16–19). However Sakurai’s result for Xe only serves as supporting but indirect evidence for the existence of beyond \( \rho(p) \) factors present in measured CPs. Other factors such as electron correlation and experimental error may play a role.

It would be interesting to see if the measured individual subshell triply differential cross sections (TDCS)—obtained from the results of photoelectron spectroscopy integrated over the ejected electron angles (see [17, 27, 33]) to obtain DDCS, which are then transformed into CP via the corrected RKJ formulas,—agree with the present S-Matrix-derived CP or with those of Biggs. If the differences around the maximum amplitude between S-Matrix and Biggs beyond the K-shell CP are real, the present results would be a first step in quantifying these differences; this appears to be considerably systematic. Such a result would indicate that expressions of the form \( f(pdp) \) do not completely describe the content of a CP even if it is obtained from a pure DDCS or TDCS Compton peak that is free of any overlap with the infrared divergence or any resonances. If this
discrepancy is a beyond momentum distribution effect it does not appear to be so large that it would prevent one from using CP data to estimate electron distributions and populations in matter and relate it to electron wavefunctions. However a more explicit characterization of such an effect would improve the accuracy of ones interpretation of CP results.

From the present results, it is clear that the higher the incident photon energy, the more options one has for obtaining a separate Compton peak from the full DDCS spectrum. This is especially true for measuring TDCS since IA requirements are greater than for DDCS [17]. Resonances cannot occur at energies greater than the binding energy of the K-shell electrons of any atom. One can more effectively shift the Compton peak away from any resonances by decreasing $\theta$ while maintaining $p_{\text{fin}}/|\vec{k}| < 1$. Here, the small angle RKJ formula can be used in place of the rather complicated full kinematic one.

For any given atomic shell from which an electron is ejected during the Compton process, the successful extraction of a CP from a full DDCS spectrum improves with an increasing momentum transfer. The momentum transfer is maximized at $\theta = 180^\circ$, which reduces $p_{\text{fin}}/|\vec{k}|$; however, the RKJ error is the largest at $\theta = 180^\circ$. For heavy atoms, one can use the high energy approximation RKJ correction for the $\omega_i > 1\text{MeV}$ range. Therefore, the correction of the RKJ error could be a useful tool for obtaining the CP from a full-spectrum DDCS. Further, equation (32) can be reversed to obtain a Compton peak from the theoretical CP. This, along with the infrared rise (LET) code, can be used to analyze QED contributions in a measured DDCS or TDCS spectrum.

6. Conclusions

An increased accuracy for the CP extracted from photon scattering DDCS was achieved by correcting the RKJ expression using NR hydrogen-like wavefunctions in addition to using relativistic kinematic factors. This method works because the relativistic and screening factors largely cancel in such expressions. Further, the simplified small angle and the high-energy forms of the RKJ correction formulas yielded good results within their respective regimes of validity.

The widely accepted requirement $p_{\text{fin}}/|\vec{k}| < 1$ for the validity of IA is not a sufficient requirement for prediction for when an accurate CP can be successfully obtained from a DDCS spectrum. There were instances where $p_{\text{fin}}/|\vec{k}| < 0.1$ was met; however, the RKJ error exceeded 30%. One reason for this is that the RKJ error is strongly $\theta$ and $l$ quantum number dependent, but not strongly dependent on $\omega_i$. In a full DDCS spectrum, one can meet the requirement $p_{\text{fin}}/|\vec{k}| < 1$ and still overlap between the Compton peak with the infrared divergence and/or with resonances. The best way to achieve a pure Compton peak is to measure the DDCS spectrum at the highest possible incident photon energy because a valid CP can only be obtained from a pure Compton peak.

Even though the corrected RKJ expression greatly reduced the differences between CP derived from RIA and those of Biggs [26], good results over the entire electron momentum distribution for CP derived from S-Matrix were only achieved for the K-shell. For all beyond K-shell cases tested, substantial differences ranging from about 5%–12% around $p_{\text{min}}=0$ occurred. The differences around the rest of the CP were generally small to moderate, and inclusion of the RKJ correction improved those results.

Further work is required to ascertain discrepancies beyond the K-shell S-Matrix CP around where $p_{\text{min}}=0$. One approach to help resolve this issue would be to obtain a single subshell DDCS by observing the energy distribution of the ejected electron from photon atom scattering experiments to obtain TDCS at a sufficiently high $\omega_i$ such that one can isolate a pure Compton peak; this in turn can be transformed into a CP and be compared to present results. Thus, this may help to establish the validity of the present S-matrix beyond K-shell results.

As a theoretical approach to resolve this issue, one may attempt to extract the factor(s) in the NR QED formula that describe the Compton peak region of the DDCS spectrum and isolate the relevant beyond K-shell terms that account for the CP region around where $p_{\text{min}}=0$. If successful the isolation of such a factor can provide a useful tool for the evaluation and quantitation of CP features that go beyond what is contained in equation (2) or (22) which are based on a simple momentum distribution function.

A possible future project would be to derive fully relativistic expressions to obtain a CP from DDCS similar to those in appendix D for L and M shell cases. The present RKJ correction based on NR wavefunctions does not consider the $j$ (spin orbit) dependence of the RKJ error. It would be of interest to compare such theoretical CPs to those extracted from measurements of photoelectron energy distributions.

Another possible future project would be to consider correcting RKJ-like expressions based on IA for other collision processes such as electron–atom and proton–atom collisions. This is of interest to anyone who uses IA and the RKJ form of IA for their research.
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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Appendix A. Dirac large and small component K-shell Fourier transformed wavefunctions

The K-shell large component wavefunction is given by

$$G_{1n/2}(p) = (2\alpha Zm)^{1/2} C_{1n/2}^+ \frac{\sin\left[\left(\gamma + 1\right)\tan^{-1}\left(\frac{p}{\alpha Zm}\right)\right]}{p^2 + (\alpha Zm)^2 \gamma^{n+1/2}},$$  \hspace{1cm} (A1)

and the corresponding small component wavefunction is

$$F_{1n/2}(p) = \frac{(2\alpha Zm)^{1/2} C_{1n/2}^-}{\gamma} \left[\frac{\sin\left[\gamma \tan^{-1}\left(\frac{p}{\alpha Zm}\right)\right]}{p^2 + (\alpha Zm)^2 \gamma^{n+1/2}} - \frac{\cos\left[\left(\gamma + 1\right)\tan^{-1}\left(\frac{p}{\alpha Zm}\right)\right]}{p^2 + (\alpha Zm)^2 \gamma^{n+1/2}}\right]$$  \hspace{1cm} (A2)

where

$$C_{1n/2}^\pm = \frac{\Gamma(\gamma)}{4\pi} \left[1 \pm \zeta\frac{1}{\gamma \Gamma(2\gamma - 1)}\right]^{1/2}, \quad \zeta = 1 + \left[1 + \left(\frac{\alpha Z}{\gamma}\right)^2\right]^{-1/2}. \hspace{1cm} (A3)$$

The above Fourier-transformed large and small component wavefunctions are obtained using a standard mathematical approach. This is achieved by starting with the K-shell radial Dirac wavefunctions, which are obtained from equation (14.39) in [34]. They are then Fourier transformed by applying

$$G(p) = \frac{1}{2\pi} \int_0^\infty r^2 G(r) e^{-ipr} dr$$  \hspace{1cm} (A4)

where

$$e^{-ipr} = \sum_{l=0}^{\infty} (2l + 1) R_l^2 (pr) P_l (\cos \theta),$$  \hspace{1cm} (A5)

with \(l = 0\) for the large component and \(l = 1\) for the small component.

The resulting integrals are solved using

$$\int_0^\infty x^{\mu-1} e^{ip\omega x} dx = \Gamma(\mu)(p^2 + q^2)^{-\mu/2} e^{-iq\tan^{-1}(q/p)}$$  \hspace{1cm} (A6)

which is obtained from equation (3), page 318 in [35].

Appendix B. Nonintegrated form of \(X^{rel}\)

$$X^{rel}(\omega, \theta, p, \phi) = 2 + F([E(p) - W - f(p, \gamma)]^{-1} - [E(p) - W - f(p, \gamma)]^{-1}) \hspace{1cm} (B1)$$

$$f(p, \phi) = D(p) + H(p) \cos \phi.$$  \hspace{1cm} (B2)
Appendix C. Integration of $X^{rel}(\omega, \theta, p, \phi)$ over $\phi$ and $p$ yields

$$X^{rel}(\omega, \theta, p_{min}) = \frac{R}{R^f} + \frac{R^f}{R} + 2m^2\left(\frac{1}{R} - \frac{1}{R^f}\right) + m^4\left(\frac{1}{R} - \frac{1}{R^f}\right)^2,$$

(C1)

Here,

$$R = \omega_0 [E(p_{min}) - D(p_{min})],$$

(C2)

$$R^f = R - \omega_0 W,$$

(C3)

$$E(p_{min}) = (p^2_{min} + m^2)^{1/2},$$

(C4)

and

$$D(p_{min}) = (\omega_0 - \omega_0 \cos \theta)p_{min} / |k|.$$  

(C5)

Appendix D. K-shell fully relativistic Compton profile

The following expression for the Fourier-transformed relativistic K-shell CP—in the form of a rapidly converging infinite series expansion—is functionally similar to equation (3) and is derived from the K-shell Dirac large and small component wavefunctions; see equations (A1)–(A3). This equation is given by

$$f_{rel}^{\text{large}}(p_{min}) = \frac{(2\alpha Zm)^{\gamma + 1} \Gamma^2(\gamma)}{4\pi^2 \Gamma(2\gamma - 1)(\gamma + 1)(\gamma + 2)(\gamma + 3)} \times \left[ \frac{\alpha_s^{(1)} + \alpha_f^{(1)}}{[p_{min}^2 + (\alpha Zm)^2]^{\gamma + 1}} + p_{min}^2 (\alpha_s^{(2)} + \alpha_f^{(2)}) + [p_{min}^2 + (\alpha Zm)^2]^{\gamma + 2} + \cdots \right],$$

(D1)

$$\alpha_s^{(1)} = 3 + \frac{307\gamma}{30} + \frac{117\gamma^2}{90} + \frac{263\gamma^3}{45} + \frac{4\gamma^4}{9} - \frac{11\gamma^5}{90} + \frac{13\gamma^6}{90} + \frac{2\gamma^7}{45},$$

(D2)

$$\alpha_f^{(1)} = \frac{14}{15} + \frac{86\gamma}{45} + \frac{7\gamma^2}{30} - \frac{9\gamma^3}{5} - \frac{7\gamma^4}{6} - \frac{7\gamma^5}{30} + \frac{\gamma^6}{10} + \frac{\gamma^7}{45},$$

(D3)

$$\alpha_s^{(2)} = -\frac{57\gamma}{45} - \frac{527\gamma^2}{90} - \frac{967\gamma^3}{90} - \frac{437\gamma^4}{45} - \frac{188\gamma^5}{45} - \frac{43\gamma^6}{90} + \frac{17\gamma^7}{45} + \frac{2\gamma^8}{45},$$

(D4)

$$\alpha_f^{(2)} = -\frac{14}{15} + \frac{128\gamma}{45} + \frac{193\gamma^2}{90} - \frac{141\gamma^3}{90} + \frac{46\gamma^4}{15} - \frac{7\gamma^5}{5} - \frac{\gamma^6}{30} + \frac{11\gamma^7}{90} + \frac{\gamma^8}{45}. $$

(D5)

Subscript $g$ represents the large component and subscript $f$ the small component corresponding to the $\gamma$ polynomials. Here, both the large and small components are described by the same function, and they differ only in the values of the $\alpha_s^{(1)}$ and $\alpha_f^{(1)}$ polynomials.

The above equation for $f_{rel}^{\text{large}}$ is obtained using the following formula for the expansion of $\tan^{-1} x$.

$$\tan^{-1} x = \frac{x}{(1 + x^2)^{1/2}} \sum_{k=0}^{\infty} \frac{(2k)!}{2^{2k}(k!)^2(2k + 1)} \left(\frac{x^2}{1 + x^2}\right)^k,$$

(D6)

where $x = p_{min} / (\alpha Zm)$. When $x = p_{min} / (\alpha Zm) = 2.17$, which corresponds to $p_{min} = 200$ for uranium, this series is about 95% converged after three terms of the above expansion are added. When $p_{min} = 100$, which is the highest value for Q in Biggs [26] and corresponds to $p_{min}$ in the present work, the convergence is 96.5% after two terms and 99.7% after three terms are added.

The expansion is completed using the fast converging infinite series (if $y < 1$) expansions for $\sin^2 y$, where $y$ is equal to the arctangent-containing arguments present in $G^2$ from (A1) and $F^2$ from (A2). The final expression is then obtained using the methods of elementary calculus (integration by parts, change of variables, etc.)

Equation (3) can be recovered by taking the NR limit ($\gamma \rightarrow 1$) of equations (D1)–(D5)

$$\lim_{\gamma \rightarrow 1} f_{rel}^{\text{large}}(p_{min}) = \frac{2^5(\alpha Zm)^3}{4\pi \Gamma(1)(4 \cdot 3 - 2)} \left[ \frac{1}{[p_{min}^2 + (\alpha Zm)^2]^2} - \frac{32p_{min}^2}{[p_{min}^2 + (\alpha Zm)^2]^3} \right].$$

(D7)
As $\gamma \to 1$, $\alpha_1^{(1)} \to 32$, and $\alpha_1^{(2)} \to -32$, whereas $\alpha_2^{(1)} = \alpha_2^{(2)} = 0$.

Each sum corresponding to $p_{\text{min}}^2$ and all terms of higher powers of $p_{\text{min}}$ can be shown to go to exactly zero in this NR limit.

In D1 of figure 20, the uranium K-shell CP obtained from equations (D1)–(D5) that only includes terms up to $p_{\text{min}}^2$ is represented by $\text{anlJ}_{\text{rel}}$ is compared to $\text{J}_{\text{rel}}$, which is obtained by the numerical integration of equation (22), wherein $p_{\text{min}}$ is in terms of equation (A1)–(A3). Further comparisons are drawn with the NR values represented by $\text{J}_{\text{NR}}$, using equation (3). $\text{anlJ}_{\text{rel}}$ and $\text{J}_{\text{rel}}$ are in good agreement with each other, and they differ by less than 1% at the peak maximum, whereas $\text{J}_{\text{NR}}$ has a considerably greater maximum magnitude and is much sharper than $\text{J}_{\text{rel}}$. The present CP results are compared with the Dirac–Hartree–Fock results of Biggs [26] ($\text{J}_{\text{Biggs}}$). As expected, the Biggs CP values are within approximately 1% of the present relativistic Coulombic results, as the screening contributions are nearly negligible for the K-shells of heavy atoms. The analytic large component of the CP $\text{anlJ}_3$ and the numerical $\text{J}_{3}$ are in good agreement (Figure 20 D2), whereas the maximum amplitude for the analytic small component $\text{anlJ}_2$ is approximately 5.5% lower than the numerical result $\text{J}_2$ (figure 20 D3).

When $Z = 62$, the error in $\text{anlJ}_2$ decreases to 1.35%, whereas the errors for $\text{anlJ}_3$ and $\text{J}_3$ are negligible. The errors in $\text{anlJ}_1$ and $\text{J}_1$ increase to $\sim 2.05%$ and 14.2%, respectively, when $Z = 120$; however, the errors almost exactly cancel, resulting in a 0.1% error in $\text{anlJ}_2$. As $Z$ increased above 120, the errors increased progressively. Although equation (D1)–(D5) converges very rapidly, one can achieve greater accuracy for $\text{anlJ}_2$ by performing an infinite series expansion of $\sin[\gamma + 1] \tan^{-1}(p/(\alpha Z m))$, $\sin[\gamma \tan^{-1}(p/(\alpha Z m))]$, and $\cos[(\gamma + 1) \tan^{-1}(p/(\alpha Z m))]$ beyond $p_{\text{min}}^2$.

$\text{anlJ}_2$ contributes approximately 6.5% to the uranium K-shell CP at a maximum, and the contribution increases to 14.5% when $Z = 120$. When $Z$ is high, this small component contribution significantly influences the shape of the CP by making it flatter around $p_{\text{min}} = 0$ and increasing the amplitude at the extremes.
Appendix E. $S_{nl}$ expressions for M and N shell CP

\[
S_{30} = \frac{p_{\text{fac}}}{4} \left( \frac{2p_{\text{fac}}^2 \Delta Z m (\alpha Zm)^2}{5 + 2445p_{\text{fac}}^2 \Delta Z m (\alpha Zm)^4} + 11487.83 \right) + 314072.78 \quad \text{(E1)}
\]

\[
S_{31} = \frac{p_{\text{fac}}}{8} \left( \frac{p_{\text{fac}}^2 \Delta Z m (\alpha Zm)^2}{17.280} + \frac{p_{\text{fac}}^2 \Delta Z m (\alpha Zm)^4}{15.552} + 23(\alpha Zm)^6 \right) + 9709.760 \quad \text{(E2)}
\]

\[
S_{32} = \frac{p_{\text{fac}}}{10} \left( \frac{p_{\text{fac}}^2 \Delta Z m (\alpha Zm)^2}{1800} + \frac{p_{\text{fac}}^2 \Delta Z m (\alpha Zm)^4}{270} + 17.010 \right) + \frac{31(\alpha Zm)^6}{122472} \quad \text{(E3)}
\]

\[
S_{42} = \frac{16p_{\text{fac}}^4 \Delta Z m (\alpha Zm)^2}{5} + \frac{2p_{\text{fac}}^2 \Delta Z m (\alpha Zm)^4}{101760} + \frac{167p_{\text{fac}}^2 \Delta Z m (\alpha Zm)^6}{376200} + \frac{737280}{322560} \quad \text{(E4)}
\]

\[
S_{43} = \frac{120p_{\text{fac}}^4 \Delta Z m (\alpha Zm)^2}{12} + \frac{181p_{\text{fac}}^2 \Delta Z m (\alpha Zm)^4}{573440} + \frac{3p_{\text{fac}}^2 \Delta Z m (\alpha Zm)^6}{286720} + \frac{10321920}{4128768} \quad \text{(E5)}
\]

equation (39), along with the equations for $S_{30}$, were obtained by the Fourier transform of NR hydrogen-like wavefunctions (see equations (A4) and (A5)) followed by integration methods based on elementary calculus.

Appendix F. Fully relativistic deltas

One can obtain explicit formulas for the fully relativistic K-shell $\Delta_1$ and $\Delta_2$ using equations (11)–(30) along with equations (D1)–(D5). The result is

\[
\frac{\Delta \rho}{\Delta \rho_{\text{rel}}}(r) = \int_{r_{\text{min}}}^{\infty} \frac{\rho(p)}{E(p)} \frac{\rho_0(p, \rho_{\text{min}})}{\rho_0(r, \rho_{\text{min}})} \frac{dE}{dr} \frac{1}{r^2} \left( \frac{p_{\text{min}}}{E(p)} \right),
\]

\[
\frac{\Delta \rho}{\Delta \rho_{\text{rel}}}(r) = \int_{r_{\text{min}}}^{\infty} \frac{\rho(p)}{E(p)} \frac{\rho_0(p, \rho_{\text{min}})}{\rho_0(r, \rho_{\text{min}})} \frac{dE}{dr} \frac{1}{r^2} \left( \frac{p_{\text{min}}}{E(p)} \right),
\]

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References

[1] Ribberfors R 1975 Phys. Rev. B 12 2067
Ribberfors R 1975 Phys. Rev. B 12 3136
[2] Eisenberger P and Reed W A 1974 Phys. Rev. B 9 3327
[3] Manninen S, Pukkari T and Kajante K 1974 Phys. Mag. 29 167
[4] Spies R and Bell F 1988 Z. Phys B Condensed Matter 70 163
[5] Sakurai H, Ota H, Tsuji N, Itou M and Sakurai Y 2011 J. Phys. B 44 065001
[6] Jaiswal P and Shukla A 2007 Phys. Rev. A 75 022504
[7] Ahuja B L, Sharma M and Bross H 2007 Phys. Status Solidi B 244 642
[8] Nara H, Kobayasi T and Shindo K 1984 J. Phys. C 17 3967
[9] Mackinnon A and Kramer B 1980 J. Phys. C 13 37
[10] Panda B K, Mahapatra D P and Padhi H C 1990 Phys. Stat. Sol. 138 261
[11] Hanssen N K, Pattison P and Schneider J R 1987 Z. Phys. B 66 305
[12] Dashora A, Marwal A, Soni K R and Ahuja B L 2010 Pramana J. Phys. 74 1017
[13] Raykar V, Sahariya J and Ahuja B L 2013 Rad. Phys. Chem. 87 37
[14] Mund H S, Sahariya J and Ahuja B L 2014 Rad. Phys. Chem. 96 148
[15] Suric T 1992 NIMA 314 240
Pratt R H, Lajohn L A, Floscuc V, Suric T, Chatterjee B K and Roy S C 2010 Rad. Phys. Chem. 79 124
Chatterjee B K, Roy S C, Suric T, Lajohn L A and Pratt R H 2007 NIMA 580 228
[16] Bergstrom P M, Suric T, Pisk K and Pratt R H 1995 Phys. Rev. A 48 1134
[17] Kaliman Z, Suric T, Pisk K and Pratt R H 1998 Phys. Rev. A 57 2683
[18] Huotari S H, Hamalainen K, Manninen S, Kaprzyk S, Bansil A, Caliebe W, Budlaps T, Honkimaki V and Suortti P 2000 Phys. Rev. B 62 7956
[19] Issolah A, Garreau Y, Levy B and Loupias G 1991 Phys. Rev. B 44 11029
[20] LaJohn L A 2010 Phys. Rev. A 81 043404
[21] Kane P P 2006 Rad. Phys. Chem. 75 2195
[22] Pradoux M, Meunier H, Avan M and Roche G 1977 Phys. Rev. A 16 2022
[23] Gopal S S and Sanjeevaiah B 1980 J. Phys. B 13 273
[24] Toye W C and Johnston P N 1998 Appl. Rad. and Iso. 49 815
[25] Bell F 1989 J. Phys. B 22 287
[26] Biggs F, Mendelsohn L B and Mann J B 1975 Atomic Data Nuclear Data Tables 16 201
[27] Florescu V and Pratt R H 2009 Phys. Rev. A 80 033421
[28] Cromer D T and Waber J T 1971 Comp. Phys. Commun. 2 107
[29] Qiao C K, Chi H C, Zhang L, Gu P, Liu C P, Tang C J and Huang K N 2020 J. Phys. B 53 075002
[30] Low F E 1958 Phys. Rev. 10 974
[31] Pratt R H and Lee C M 1977 PRA 16 1733
[32] Rosenberg L 1991 PRA 44 2949
[33] Bergstrom P M and Pratt R H 1997 Rad. Phys. Chem. 50 3
[34] Bethe H A and Salpeter E E 1957 Quantum Mechanics of One and Two Electron Systems (Berlin Heidelberg: Springer)
[35] Gradshteyn I S and Ryzhik I M 1980 Table of Integrals, Series, and Products (New York: Academic Press, INC.)