Contribution of bound-electron pair production to the dispersion relation for Delbrück scattering

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In photon-atom scattering the customary partitioning of the elastic scattering amplitude into Rayleigh and Delbrück amplitudes (as well as nuclear amplitudes) in the single-electron formalism involves summations over complete sets of intermediate electron states in the atomic potential. This leads to the Rayleigh amplitude which is usually compared with experiment. However, another consequence of the partition is that the total cross section for bound-electron pair-production into all bound states, regardless of occupation, is included in the optical theorem for the imaginary part of the forward Delbrück amplitude. The corresponding real part of the forward Delbrück amplitude can be obtained through the use of a dispersion relation. We show that for $Z=92$ the inclusion of the bound-electron pair-production cross section leads to a contribution to the real part of forward Delbrück amplitude, which can be as much as $\approx 12\%$ of the Born approximation result, for photon energies near the pair-production threshold. This bound-electron pair-production contribution is therefore comparable in magnitude to the corrections due to Coulomb and screening effects in the ordinary pair-production cross section (electron in continuum). The net correction to Born approximation is small well below threshold, significant well above threshold. [S1050-2947(99)07310-2]

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I. INTRODUCTION

Coulomb and screening effects in Delbrück scattering, the scattering of light by an electromagnetic field, are a subject of ongoing theoretical interest. Experimental results for (large-angle) scattering from high-Z atomic targets at 1.33 MeV [1,2] appear to be in agreement with theory if the available Born approximation results [3–5] are used to describe the Delbrück amplitude (they are not in agreement if the Delbrück amplitude is neglected altogether). However, results at 2.754 MeV are not in agreement with theory even when the Delbrück amplitude is included in the Born approximation, and it has been argued this indicates the importance of Coulomb effects in the Delbrück amplitude there [6,7].

There is still no complete S-matrix calculation of the Delbrück scattering amplitude, including effects beyond Born approximation, though analogous S-matrix calculations have been done numerically for other processes, such as Rayleigh scattering [8–10], Compton scattering [11], and bremsstrahlung [12], A formalism has been given [13], (based on the formalism of Wichmann and Kroll [14] for vacuum polarization), and some limited numerical results and partial calculations have been reported [15] within this formalism. This calculation is complicated both numerically and in principle, since the amplitude describing this process is divergent and requires performing (external-field) renormalization. (There are calculations which involve limiting approximations, e.g., assumptions of small angles and high energies [16,17].) For a detailed discussion of the current situation we refer the reader to the recent review article [18], which builds on an earlier review [19].

For forward-angle Delbrück scattering one can use the optical theorem (in an expansion in the fine-structure constant α) and a dispersion relation to obtain the scattering amplitude from knowledge of the lower-order total cross sections for pair production. Though a discussion of forward-angle Delbrück scattering takes us away from the situations of present experimental interest, it still serves as a useful check for a future more general calculation.

Rohrlich and Gluckstern [3] calculated the forward Delbrück scattering amplitude in the Born approximation by using the optical theorem to relate the imaginary part of the amplitude to the total cross section for pair production (evaluated in the Born approximation), and using a dispersion relation to then obtain the real part. (They also derived the same result for the forward Delbrück scattering amplitude by evaluating the corresponding Feynman graphs.)

One can proceed to include effects beyond the Born approximation by replacing the results for the pair-production cross section in the Born approximation with better estimates for the pair-production cross section, including Coulomb and screening effects. This directly gives the imaginary part of the forward Delbrück amplitude, including Coulomb and screening effects, and the dispersion relation gives the real part. Solberg *et al.* [20] obtained the corrections to the Born result for the forward Delbrück amplitude due to Coulomb and screening effects in the ordinary (electron in continuum) pair-production total cross section using this procedure (though, as will be discussed, their screening corrections were not accurate for photon energies near the pair-production threshold).

However, the Born approximation completely neglects bound-electron pair production, which should also be considered. Furthermore, given the usual partitioning of the elastic-scattering amplitude (see next section), one should consider the total cross section for bound-electron pair production into all bound states, regardless of occupation (and not just the physically accessible unoccupied bound states). We will show that these corrections can be comparable with the corrections due to Coulomb and screening effects in ordinary pair production in the energy regime around the pair-production threshold and below, while they are becoming unimportant at higher energies.

In Sec. II the elastic amplitude is partitioned into Rayleigh and Delbrück amplitudes in the single-electron formalism, describing elastic scattering off the bound atomic electrons and off virtual electron-positron pairs, respectively, together with amplitudes describing elastic scattering off the nucleus. The optical theorem and dispersion relation are written for each amplitude separately, corresponding to this partitioning. In Sec. III numerical results are given for the contribution of the bound-electron pair-production total cross section to the forward Delbrück amplitude in the case of scattering from neutral ground-state uranium ($Z=92$). This contribution is compared with the corrections due to Coulomb and screening effects in the ordinary pair-production cross section. Conclusions are presented in Sec. IV.

II. PARTITIONING OF THE ELASTIC SCATTERING AMPLITUDE

The total amplitude for coherent elastic photon-atom scattering is traditionally partitioned into Rayleigh, Delbrück, and nuclear amplitudes, which can be thought of as describing scattering off the atomic bound electrons, off virtual electron-positron pairs in the atomic field, and off the nucleus, respectively. In going to a single-electron formalism [21], one has written the Rayleigh amplitude for a given bound state as a sum over all possible intermediate states, including other occupied bound states and negative energy states. By writing the Rayleigh amplitude in such a way one has defined a partitioning scheme for the Rayleigh amplitude, and for consistency the same partitioning scheme must be used for the Delbrück amplitude. This in particular implies that the Delbrück amplitude must be written so as to include the influence of all virtual electron-positron pairs, even when the electron is created in an occupied bound state of the atomic potential. Current *S*-matrix predictions for Rayleigh scattering [10] use this partitioning (which is regarded as attractive since the ability to sum over all intermediate states in closed form allows one to solve the inhomogeneous wave equation for a perturbed orbital instead of explicitly constructing the Green's function as a summation over the states).

This partitioning scheme implies that there will be unphysical spurious transitions present in the separate partitioned amplitudes, which violate the Pauli principle. Of course such spurious transitions must cancel when the partitioned amplitudes are added to obtain the total coherent amplitude, on which the physical observables depend. It is well known that such a phenomena occurs in the individual Rayleigh amplitudes defined for each of the bound electrons for the case of multielectron atoms and ions. The Rayleigh amplitude for one of the occupied bound states n will contain spurious resonances corresponding to virtual transitions to another occupied bound state m. Similarly, the Rayleigh amplitude for the occupied bound state m will contain spurious resonances corresponding to virtual transitions to the occupied bound state n. In summing to get the total Rayleigh amplitude the spurious resonances corresponding to transitions between occupied states cancel.

Now, write the optical theorem involving the single-particle partitioned Rayleigh amplitude for one of the occupied bound states n [21] as

$$\mathrm{Im}\, R_n = \frac{\omega}{4\pi c}(\sigma_n^{PE} + \sigma_n^{BBT+} - \sigma_n^{BBT-} - \sigma_n^{BPP}), \qquad (1)$$

where ω is the photon energy, σ_n^{PE} is the photoeffect total cross section for the bound state n, σ_n^{BBT+} is the total cross section for upward bound-bound transitions starting from the bound state n, σ_n^{BBT-} is the total cross section for downward bound-bound transitions starting from the bound state n, and σ_n^{BPP} is the bound-electron pair-production total cross section with the electron being created in the bound state n. As discussed in [10] the subtraction of the bound-electron pair-production cross section in Eq. (1), needed in the single-electron formalism for a complete set of intermediate states, is necessary in order that the real part of the Rayleigh amplitude, defined through the dispersion relation, will have a finite high-energy limit. To get the total Rayleigh amplitude one sums over all occupied bound states n.

In this partitioning scheme the optical theorem written for the Delbrück amplitude is

$$\mathrm{Im}\, D = \frac{\omega}{4\pi c}(\sigma^{PP} + \sigma^{BPP}), \qquad (2)$$

where σ^{PP} is the ordinary (electron in continuum) pair-production total cross section, and σ^{BPP} is the bound-electron pair-production total cross section, summed over production into all bound states, regardless of occupation. In summing to get the total coherent amplitude, for which we can again write the optical theorem for the imaginary part [that being just the sum of Eq. (1), summed over all occupied bound states n, and of Eq. (2)] we see that the contribution of the total bound-electron pair-production cross section for production into the *occupied* bound states cancels, as it should.

III. NUMERICAL RESULTS AND DISCUSSION

We write the forward Delbrück amplitude $D=D(\omega,\theta=0)$ in terms of a Born term D^{Born}, a correction term due to Coulomb and screening effects in the ordinary (electron in continuum) pair-production cross section ΔD^{PP}, and a correction term due to the inclusion of the bound-electron pair-production cross section ΔD^{BPP},

$$D(\omega,\theta=0) = D^{Born} + \Delta D^{PP} + \Delta D^{BPP}. \qquad (3)$$

Note that the Born term can be obtained from the ordinary pair-production cross section in the Born approximation (given by [22], and in terms of simple expansions by Maximon [23]). It can also be obtained directly through the evaluation of the appropriate lowest-order Feynman graphs [3–5].

The corrections ΔD^{PP} to the Born result obtained by using the ordinary pair-production cross section, but including Coulomb and screening effects, have been investigated by Solberg *et al.* [20], who gave separately the corrections due to Coulomb and screening effects. This was based on previous work on the Coulomb [24,25] and screening [26,27] corrections to ordinary pair production. While the Coulomb corrections reported in these works are valid throughout the threshold regime, the screening corrections (based on screening corrections to the Born term and shifted Coulomb values to account for screening corrections to the Coulomb term) are not valid for low photon energies close to the pair-production threshold ($\omega \lesssim 2.5\ mc^2$ for $Z=92$) [26]. Since the threshold region is our region of interest, we will use the pair-production tabulation of Hubbell *et al.* [28] to calculate the total correction due to Coulomb and screening effects in ordinary pair production for comparison with our results for corrections due to the bound-electron pair-production cross section. At low photon energies, near the pair production threshold, the tabulation of Hubbell *et al.* [28] uses screening corrections based on the numerical work of Tseng and Pratt [29,30], which are then matched to the screening corrections of Øverbø [26,27] so as to accurately account for screening throughout the threshold regime. The Coulomb corrections [24,25] are also included, as are radiative corrections [31,32] which are small ($\approx 1\%$ or less).

We consider the correction ΔD^{BPP}, defined as the correction to the forward amplitude due to bound-electron pair production into all bound states. The imaginary part of the correction is given directly by

$$\operatorname{Im} \Delta D^{BPP} = \frac{\omega}{4\pi c}(\sigma^{BPP}), \tag{4}$$

where $\sigma^{BPP}=\sigma^{BPP}(\omega)$ is the total cross section for bound-electron pair production with production into all bound states, regardless of occupation. The real part of the correction is obtained by use of the dispersion relation

$$\operatorname{Re} \Delta D^{BPP} = \frac{\omega^2}{2\pi^2}\, \mathrm{P}\int_{2mc^2-E_K}^{\infty} \frac{\sigma^{BPP}(\omega')}{\omega'^2-\omega^2} d\omega', \tag{5}$$

where P indicates that the principal value of the integral should be taken. Note the lower limit of the integral is $2mc^2-E_K$ rather than $2mc^2$, where E_K is the binding energy of the *K* shell (σ^{BPP} vanishes for photon energies lower than $2mc^2-E_K$).

Though the bound-electron pair-production cross section to be used in Eqs. (4) and (5) includes production into all bound states, it is well known that production into the inner shells dominates, as in the case of bound-electron pair annihilation and photoeffect at the same energies [33–35]. We have calculated explicitly the bound-electron pair-production cross sections for production into the *K* and *L* shells. Our results for the *K* and *L* shell taken separately exhibit the expected *L* to *K* shell ratio of ≈ 0.18 (above the *L*-shell threshold) seen in photoeffect cross sections for the same *Z* at similar energies [35]. In [35] the ratio of the *L*-shell photoeffect cross section to the sum of the *M*- and higher-shell photoeffect cross sections is given for $Z=92$ as 3.105 at 1.332 MeV and as 3.090 at 0.662 MeV, quite insensitive to energy. Therefore we approximate the effect of bound-electron pair production into the *M* and higher shells by assuming a ratio of 0.06 to the *K*-shell result.

In Fig. 1 we show the real and imaginary parts of the forward Delbrück amplitude *D*, given in terms of the classical electron radius r_0, for photon energies in the range 0.5–100 MeV. This result includes both corrections due to Coulomb and screening effects in ordinary pair production, and corrections due to bound-electron pair-production. We see that the real amplitude dominates the imaginary amplitude around and below the pair production threshold, with a crossover near 7 MeV. The lowest-lying threshold for (bound-electron) pair production is shown, 0.906 MeV, corresponding to production into the *K* shell. Below 0.906 MeV the imaginary amplitude vanishes. (Note that without the inclusion of corrections due to bound-electron pair production the imaginary Delbrück amplitude vanishes below 1.022 MeV, the threshold for ordinary pair production.)

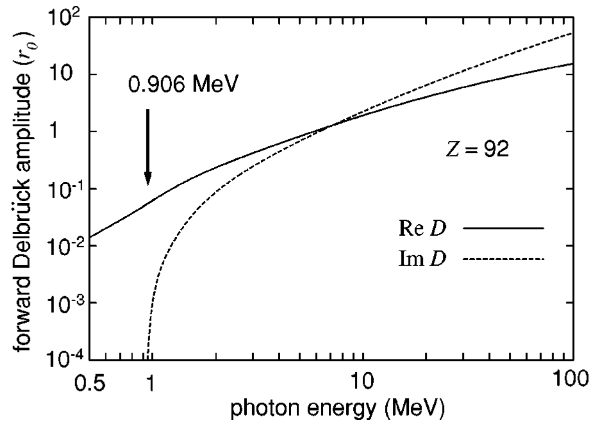

FIG. 1. Real and imaginary parts of the full forward Delbrück amplitude *D* for $Z=92$, including corrections due to Coulomb and screening effects in ordinary pair production, and due to bound-electron pair production, in terms of the classical electron radius r_0. The threshold for production into the *K* shell (0.906 MeV) is indicated, below which the imaginary amplitude vanishes.

In Figs. 2 and 3 we show the real and imaginary parts respectively of the corrections ΔD^{BPP} and ΔD^{PP}, expressed as fractions of the corresponding real or imaginary parts of the full forward Delbrück amplitude *D*. The net correction due to beyond-Born-approximation effects, being the sum of these, is also shown. At high energies, well above threshold, the correction ΔD^{BPP} becomes unimportant, and our results are in general agreement with those of [20], where only the correction ΔD^{PP} was considered.

Below 7 MeV it is effects in the real amplitude that will most affect the scattering cross section. Figure 2 shows that

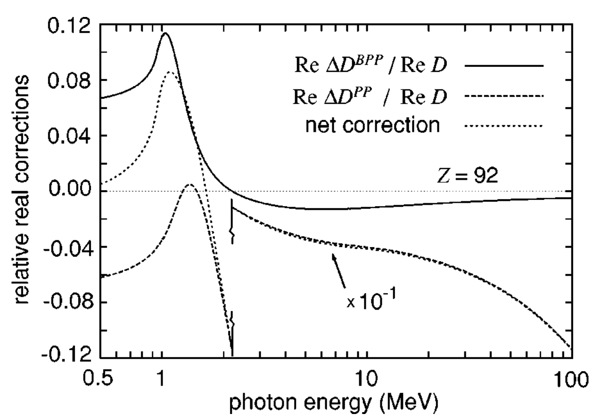

FIG. 2. Real part of the corrections ΔD^{BPP} and ΔD^{PP} for $Z=92$, given as a fraction of the corresponding real part of the full forward Delbrück amplitude *D*. The net correction, being the sum of these, is also shown. The fraction $\operatorname{Re}\Delta D^{PP}/\operatorname{Re} D$ and the net correction are shown with a multiplicative factor of 10^{-1} above 2.2 MeV, so as fit on the scale used.

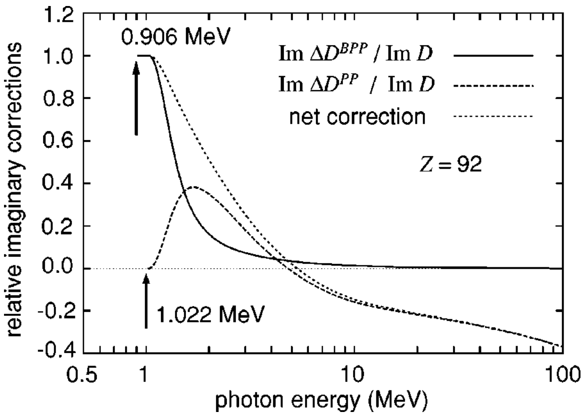

FIG. 3. Imaginary part of the corrections ΔD^{BPP} and ΔD^{PP} for $Z=92$, given as a fraction of the corresponding imaginary part of the full forward Delbrück amplitude D. The net correction, being the sum of these, is also shown. The thresholds for production into the K shell (0.906 MeV) and ordinary pair production (1.022 MeV) are indicated.

below 2 MeV the correction $\mathrm{Re}\,\Delta D^{BPP}$ is comparable with $\mathrm{Re}\,\Delta D^{PP}$, and both need to be considered. $\mathrm{Re}\,\Delta D^{BPP}$ accounts for as much as $\approx$11% of the real forward Delbrück amplitude in the threshold region. At low energies the corrections $\mathrm{Re}\,\Delta D^{BPP}$ and $\mathrm{Re}\,\Delta D^{PP}$ cancel each other, so that the Born result is accurate at the 1% level (though the Delbrück amplitude is unimportant at low energies). At somewhat higher energies $\mathrm{Re}\,\Delta D^{PP}$ is dominant, and the net correction to Born approximation is significant. It is interesting that qualitatively similar features are found in the experimental large-angle scattering results. (But note that in forward scattering $\mathrm{Re}\,\Delta D^{BPP}$ is the dominant and significant correction around 1.3 MeV.)

The primary effect of the correction $\mathrm{Im}\,\Delta D^{BPP}$ on the imaginary part of the forward Delbrück amplitude is to shift the threshold below which the imaginary part of the amplitude vanishes from 1.022 MeV (ordinary pair-production threshold) down to 0.906 MeV (threshold for production into the K shell for $Z=92$). Consequently $\mathrm{Im}\,\Delta D^{BPP}/\mathrm{Im}\,D\equiv 1$ below 1.022 MeV as bound-electron pair production is then responsible for the entire contribution of the imaginary forward Delbrück amplitude. The correction $\mathrm{Im}\,\Delta D^{PP}$ becomes comparable with $\mathrm{Im}\,\Delta D^{BPP}$ above threshold and dominates by 10 MeV.

IV. CONCLUSIONS

We have considered the corrections due to the inclusion of the bound-electron pair-production cross section (completely neglected in the Born approximation) in the optical theorem for the imaginary part of the forward Delbrück scattering amplitude. The real part is obtained via a dispersion relation. The usual single-electron partitioning of the elastic-scattering amplitude implies that the cross section for bound-electron pair production into all bound states (both occupied and unoccupied) should be included. Numerical results for the correction to the real part of the forward Delbrück amplitude due to bound-electron pair production indicate a correction as large as $\approx$12% of the Born approximation result in the region just above the pair-production threshold. (The real part of the forward Delbrück amplitude dominates in this regime.) Thus, these effects are comparable in this regime with the corrections due to Coulomb and screening effects in the ordinary (electron in continuum) pair-production cross section (they become unimportant at higher energies), and both need to be considered for energies near and below the pair-production threshold. The net correction to Born approximation is small well below threshold and significant well above threshold.

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