

All-Order Coulomb Corrections to Delbrück Scattering above the Pair-Production Threshold

J. Sommerfeldt^{1,2,*}, V. A. Yerokhin^{1,3}, Th. Stöhlker^{4,5} and A. Surzhykov^{1,2}

¹Physikalisch-Technische Bundesanstalt, D-38116 Braunschweig, Germany

²Technische Universität Braunschweig, D-38106 Braunschweig, Germany

³Max-Planck-Institut für Kernphysik, D-69117 Heidelberg, Germany

⁴Helmholtz Institute Jena, D-07743 Jena, Germany

⁵GSI Helmholtzzentrum für Schwerionenforschung GmbH, D-64291 Darmstadt, Germany



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We report calculations of Delbrück scattering that include all-order Coulomb corrections for photon energies above the threshold of electron-positron pair creation. Our approach is based on the application of the Dirac-Coulomb Green's function and accounts for the interaction between the virtual electron-positron pair and the nucleus to all orders in the nuclear binding strength parameter αZ . Practical calculations are performed for the scattering of 2.754 MeV photons off plutonium atoms. We find that including the Coulomb corrections enhances the scattering cross section by up to 50% in this case. The obtained results resolve the long-standing discrepancy between experimental data and theoretical predictions and demonstrate that an accurate treatment of the Coulomb corrections is crucial for the interpretation of existing and guidance of future Delbrück scattering experiments on heavy atoms.

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Introduction.—Classical electrodynamics is known to be linear in vacuum, which implies the absence of light-light interactions. In quantum electrodynamics (QED), however, photons can interact with each other by means of creation and annihilation of virtual electron-positron pairs. This interaction enables a class of nonlinear QED processes, including photon splitting and coalescence, as well as light-by-light and Delbrück scattering. The Delbrück scattering occupies a special place among them since it is the nonlinear QED process that can be studied most accurately in experiment [1–3].

Delbrück scattering is the elastic scattering of photons by the Coulomb field of atomic nuclei. Precise knowledge of this fundamental process can provide unique tests of the nonlinear aspects of QED theory. It is also required to analyze nuclear photon scattering experiments and to improve our quantitative knowledge of the nuclear structure. In particular, accurate predictions of the Delbrück amplitudes are needed to extract information on the static electric nuclear polarizability, the giant dipole, and isovector giant quadrupole resonances [4–6]. So far, these possibilities have not been fully explored because a sufficiently accurate theoretical description of Delbrück scattering is not available.

The most widely used approach in the region of moderate energies of 1–10 MeV is the lowest-order Born approximation as developed by Papatzacos and Mork [7]. This approximation is based upon expanding the Delbrück amplitude in the Coulomb-field strength parameter αZ , where Z is the nuclear charge and $\alpha \approx 1/137$ is the

fine-structure constant, and neglecting all terms beyond the lowest order that are usually referred to as Coulomb corrections. The Born approximation usually works well for light atoms [2,3]. However, for heavy nuclei the expansion parameter αZ is not small and the Coulomb corrections drastically change the cross section as compared to the Born approximation [2]. Moreover, the Delbrück cross section scales as Z^4 to leading order [7], making this scattering channel increasingly important for high- Z targets and allowing experiments to achieve a higher accuracy.

In order to better understand Delbrück scattering in the high- Z regime, new experiments are planned that use nuclear γ sources, Compton scattering techniques, and novel accelerator facilities that will employ gamma rays with energies above the electron-positron pair production threshold [8–13]. The necessary prerequisite for the success of these experiments is a breakthrough in the theory of Delbrück scattering, since previous calculational approaches were not adequate in the high- Z regime, as was repeatedly stressed in the literature [2,14–17]. In particular, the measured angle differential cross section for the scattering of 2.754 MeV photons off neutral plutonium atoms was found to differ from the lowest-order Born predictions by almost a factor of 2 [15]. This long-standing discrepancy has not been resolved up to now and is commonly attributed to the unknown Coulomb corrections.

Despite the considerable interest, all-order calculations of Delbrück scattering above the pair production threshold have remained an unsolved problem in theoretical physics

for at least half a century. The first steps to set up an *ab initio* theory that accounts for all orders in the Coulomb-field strength parameter for Delbrück scattering were performed by Scherdin and co-workers three decades ago [18,19]. However, due to overwhelming technical difficulties, no actual calculations for energies above the pair-creation threshold were carried out. In this Letter, we develop a novel approach to evaluate and compute Delbrück scattering amplitudes for a wide range of scattering energies including those beyond the threshold. This approach is based on the use of the Dirac-Coulomb Green's function, whose exact closed analytical form accounts for the Coulomb interaction between electrons (positrons) and a nucleus to all orders in αZ . The use of the Green's function eliminates the need for an αZ expansion but requires an accurate treatment of its poles. The latter has been done by using a modified Wick rotated integration contour. Our approach allows for accurate Delbrück calculations in the high- Z and high photon energy regime. To illustrate the application of the developed method, we present calculations for the scattering of 2.754 MeV photons by plutonium atoms. We demonstrate that by accounting for the higher-order Coulomb corrections, one can resolve the long-standing discrepancy and reproduce the experimental results by Rullhusen and co-workers [15]. In the future, such calculations can be extended to other systems and higher energies, which opens a way for testing the nonlinear aspects of QED and determining nuclear properties from x-ray scattering experiments. Relativistic units (r.u.) $\hbar = m_e = c = 1$ are used throughout this Letter, if not stated otherwise.

Theoretical background.—The Feynman diagram for Delbrück scattering is depicted in Fig. 1. Here, we follow the standard convention where the wavy lines represent the incoming and outgoing photon with wave vector \mathbf{k}_1 and \mathbf{k}_2 and polarization vector $\boldsymbol{\epsilon}_1$ and $\boldsymbol{\epsilon}_2$, and the double lines correspond to the virtual electron-positron pair in the Coulomb field of the nucleus. Each vertex \mathbf{r}_1 and \mathbf{r}_2 contributes a factor of $\sqrt{\alpha}$ to the scattering amplitude while the Dirac-Coulomb solutions for the electron and positron account for all orders in αZ .

According to the well-known Feynman correspondence rules, the amplitude for the diagram in Fig. 1 can be written as

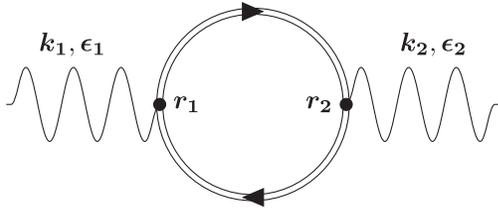


FIG. 1. Feynman diagram for Delbrück scattering to leading order in α and all orders in αZ .

$$M_{\epsilon_1, \epsilon_2}^D = \frac{i\alpha}{2\pi} \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dz' \int d^3\mathbf{r}_1 \int d^3\mathbf{r}_2 \times \text{Tr}[\hat{R}(\mathbf{r}_1, \mathbf{k}_1, \boldsymbol{\epsilon}_1) G(\mathbf{r}_1, \mathbf{r}_2, z) \hat{R}^\dagger(\mathbf{r}_2, \mathbf{k}_2, \boldsymbol{\epsilon}_2) \times G(\mathbf{r}_2, \mathbf{r}_1, z')] \delta(\omega + z - z'). \quad (1)$$

Here, $G(\mathbf{r}_2, \mathbf{r}_1, z)$ is the Dirac-Coulomb Green's function with the three-dimensional coordinate vectors \mathbf{r}_1 and \mathbf{r}_2 as well as the energy argument z . Moreover, $\hat{R}(\mathbf{r}, \mathbf{k}, \boldsymbol{\epsilon})$ is the photon-lepton interaction operator with \mathbf{k} and $\boldsymbol{\epsilon}$ being the wave and polarization vectors and ω being the energy of the incoming and outgoing photon [3].

Further evaluation of the amplitude (1) for the case when the photon energy is below the threshold for electron-positron pair production was discussed by us in Ref. [20]. However, the previous approach has to be extended for the more troublesome case of above threshold photon scattering. In what follows, therefore, we will discuss the challenges of this high energy analysis, $\omega \geq 2$ r.u., and refer for all other details to Ref. [20]. First, to get sensible results from the Feynman diagram in Fig. 1, one needs to eliminate the divergent free-loop contribution from the amplitude. As usual in bound-state QED calculations, the free diagram can be obtained by setting the nuclear charge to zero in the amplitude, see, e.g., [21]. Now, we are ready to perform the energy integration in Eq. (1) over z and z' . While the integral over z is trivial due to the Dirac delta function $\delta(\omega + z - z')$, the substitution $z' \rightarrow z' + \frac{1}{2}$ simplifies the numerical z' -integration. Indeed, as seen from Fig. 2, the starting points of the branch cuts of the Green's functions are located after this substitution at $z' = \pm 1 + (\omega/2)$ and $z' = \pm 1 - (\omega/2)$, i.e., *symmetrically* with respect to the coordinate origin. Such symmetry makes calculations more stable as shown in Ref. [20]. Along with the cuts, one can also see two sets of bound-state poles localized at $z' = (\lambda' + m)/\sqrt{(\alpha Z)^2 + (\lambda' + m)^2} + (\omega/2)$ and $z' = (\lambda + m)/\sqrt{(\alpha Z)^2 + (\lambda + m)^2} - (\omega/2)$, $m = 0, 1, 2, \dots$. Both, the branch cuts and the two sets of poles, moreover, are shifted by $\delta \rightarrow \pm i0$ off the real axis.

The infinitely close location of the poles of the Green's function to the naive integration path on the interval $z' \in (-\infty, +\infty)$, displayed in the upper panel of Fig. 2, makes the numerical evaluation of the amplitude (1) very troublesome. It is more convenient to perform the well-known Wick rotation of the contour and integrate along the imaginary axis instead. However, in contrast to the previous below-threshold calculations, the branch cuts cross the imaginary axis for photon energies $\omega \geq 2$ r.u. In order to overcome this difficulty, we follow Ref. [19] and modify the Wick-rotated contour to incorporate additional paths that go around the branch cuts (C_2) and add the residue of the integrand for the enclosed poles (C_3), see lower panel of Fig. 2. By employing this modified contour, we finally obtain

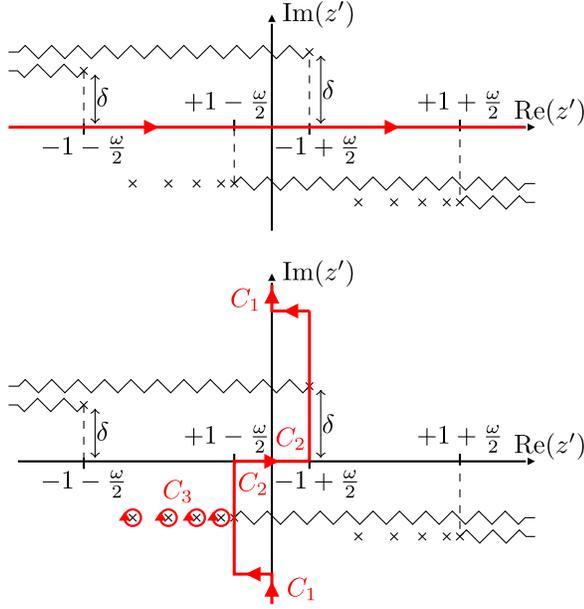


FIG. 2. Original (upper panel) and Wick rotated (lower panel) contour for the z' integration in the Delbrück amplitude (1). The modified contour consists of paths along the imaginary axis (C_1) and around the branch cuts (C_2) as well as contributions from the residue (C_3). Moreover, the branch cuts (black zigzag lines) and a finite subset of the countably infinite singularities (black crosses) of the Green's functions in Eq. (1) are shown for the case of above threshold photon energies.

$$\int_{-\infty}^{\infty} dz' f(z') = \int_{C_1, C_2} dz' f(z') - 2\pi i \sum_n \text{Res}[f, z'_n], \quad (2)$$

where for the sake of brevity, we used the notation $f(z')$ for the integrand in Eq. (1) with $\text{Res}[f, z'_n]$ being the residue of $f(z')$ at its n th enclosed pole z'_n .

The evaluation of Eq. (2) requires the calculation of the integral along the paths C_1 and C_2 as well as the summation over the residue of the poles of the integrand C_3 . The methods used to evaluate the path along the imaginary axis C_1 are identical to the case of below-threshold energies and are discussed in detail in Ref. [20]. In contrast, the integration along C_2 and the summation over the residue C_3 requires some important modifications that need to be discussed. For example, when integrating along C_2 , we find that the integrand is strongly peaked at the beginning of the branch cuts at $z' = \pm 1 \mp (\omega/2)$. To perform the integration, we use Gauss-Legendre quadrature with an enhanced density of integration points close to the peaked regions which can be achieved by the substitution $z' \rightarrow \pm u^2 + [\pm 1 \mp (\omega/2)]$. To calculate the residue C_3 , we note that the poles originate from a prefactor $\Gamma(\lambda' - \nu')$ arising in the radial components of the Green's function [21], where $\lambda' = \sqrt{\kappa'^2 - (\alpha Z)^2}$, $\nu' = \alpha Z[z' + (\omega/2)]/c'$, $c' = \sqrt{1 - [z' + (\omega/2)]^2}$, and κ' is the Dirac quantum number of one of the propagators. Therefore, to obtain

the contribution from the bound states, we simply replace this prefactor by its residue

$$\begin{aligned} \text{Res} \left[\Gamma(\lambda' - \nu'), z'_n = \frac{\lambda' + n}{\sqrt{(\alpha Z)^2 + (\lambda' + n)^2}} - \frac{\omega}{2} \right] \\ = - \frac{(-1)^n \left(1 - \frac{(\lambda' + n)^2}{(\alpha Z)^2 + (\lambda' + n)^2} \right)^{3/2}}{n! \alpha Z}. \end{aligned} \quad (3)$$

Together with the integration over the energy z' , the evaluation of the radial integrals in Eq. (1) is also a highly demanding task. This is due to the fact that after some algebra presented in Ref. [20], the integrand in Eq. (1) can be written in terms of products of Whittaker functions $M_{\alpha, \beta}(2\tilde{c}r_2)$ and $W_{\alpha, \beta}(2\tilde{c}r_1)$, where $\tilde{c} = \sqrt{1 - [z' \pm (\omega/2)]^2}$, which are fast oscillating and slowly decreasing at large radial arguments. To compute the integrals over r_1 and r_2 , we split the integrals into two parts. For small radial distances, we perform the radial integrations numerically, whereas for large distances we employ the asymptotic expansion of the Whittaker functions to calculate the integrals analytically. In contrast to the below-threshold case of Ref. [20], however, the analysis of the asymptotic representation of the Whittaker functions requires some special attention if $\omega \geq 2$ r.u. The reason for this is the second term of the asymptotic expansion of $M_{\alpha, \beta}(2\tilde{c}r_2) \propto M_1 e^{\tilde{c}r_2} + M_2 e^{-\tilde{c}r_2}$ which is always exponentially smaller than the first term for $\omega < 2$ r.u. but can be of comparable magnitude for higher energies. The radial integral including this term was also derived analytically in terms of incomplete Gamma functions. In general, the radial integration is a very time consuming task which was accomplished by utilizing a hybrid parallelization scheme at the PTB high performance cluster. This allowed us to perform a full calculation for one charge number and photon energy in approximately one week using around 200 threads.

So far, we have discussed the theory used to calculate Delbrück scattering amplitudes. With the help of these amplitudes, one can calculate the angle-differential as well as total cross sections of the Delbrück process. However, in order to compare the results of our calculations with experimental data, we have to account also for competing scattering processes. These are the Rayleigh scattering off bound atomic electrons and nuclear Thomson scattering. The Rayleigh and Delbrück scattering processes are closely related as can be readily seen in the redefined vacuum approach [22–24]. In this approach, the vacuum Fermi level in the Delbrück amplitude is shifted to include the Dirac energies of the occupied atomic shells. In practice, it implies changing the sign of the infinitesimal imaginary additions for the poles of the electron propagator corresponding to the occupied shells. The expressions for the Rayleigh amplitude are then obtained as the difference of the Delbrück amplitudes with the modified and the standard vacuum, as illustrated in Fig. 3. We have checked that

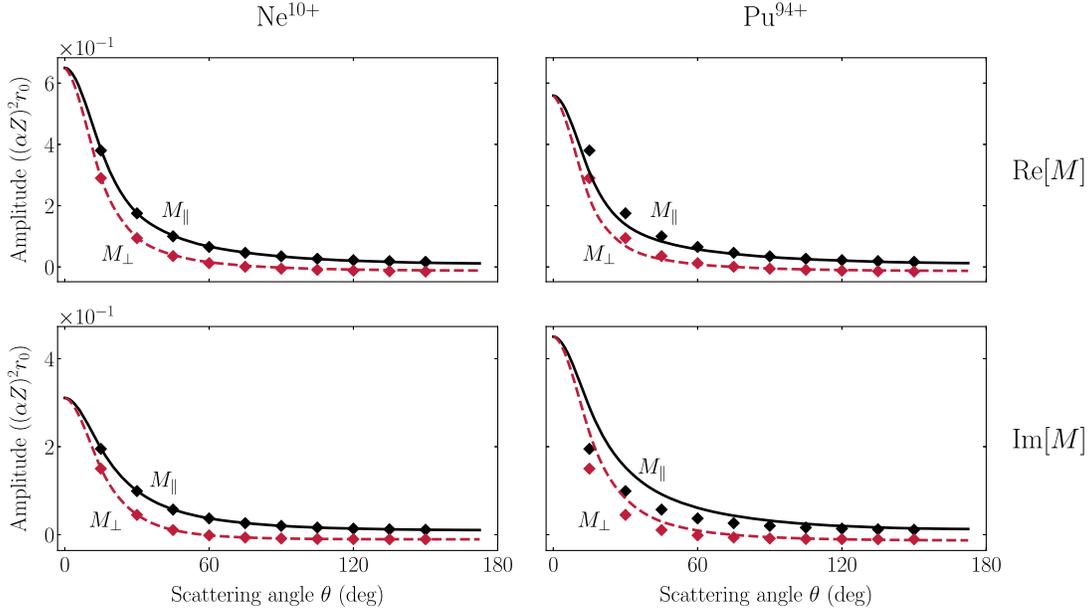


FIG. 4. Real (upper panels) and imaginary (lower panels) parts of the amplitude for Delbrück scattering (1) of 2.754 MeV photons by bare neon (left panels) and plutonium (right panels) nuclei. Calculations have been performed for linear polarization of the incoming and outgoing photons parallel (black solid line) as well as perpendicular (red dashed line) to the scattering plane. Moreover, the lowest-order Born predictions from Ref. [31] are shown (diamonds). The amplitudes are given in units $(\alpha Z)^2 r_0$, where $r_0 = 2.818$ fm is the classical electron radius.

$$\frac{d\sigma}{d\Omega} = \frac{1}{2} (|M_{\parallel}|^2 + |M_{\perp}|^2), \quad (6)$$

where $M_{\parallel/\perp}$ is the sum of the amplitudes for Delbrück, Rayleigh as well as nuclear Thomson scattering and where the incoming radiation is assumed to be unpolarized. In Fig. 5, we display this cross section together with its

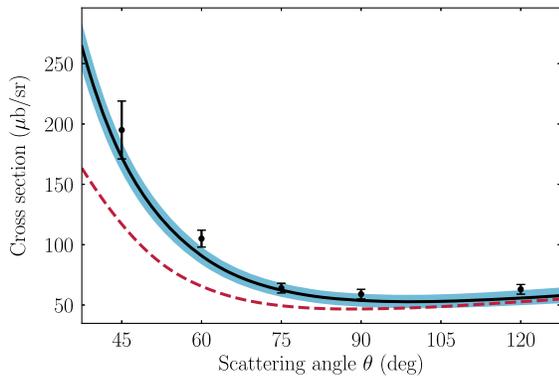


FIG. 5. Differential cross section for elastic scattering of 2.754 MeV unpolarized photons by plutonium atoms. The black dots display the experimental data from Ref. [15], the black solid line indicates the theoretical results based on all order in αZ Delbrück calculations while the shaded region shows the theoretical error. Theoretical predictions using the lowest-order Born approximation for Delbrück scattering are displayed with the red dashed line.

theoretical uncertainty and the experimental findings from Ref. [15]. Moreover, we present the theoretical predictions based on the lowest-order Born approximation for the Delbrück amplitude. As seen from the figure, the higher-order Coulomb corrections to the Delbrück process lead to a strong enhancement of the cross section for scattering angles $\theta < 90^\circ$. All-order in αZ predictions agree well with experimental data from Ref. [15], thus, solving the long standing discrepancy between experiment and lowest-order Born theory. This agreement together with the computational stability of our analysis justifies the use of the proposed method for all-order calculations of Delbrück scattering for photon energies above the pair production threshold. In the future, such calculations will be performed to plan and to analyse Delbrück scattering experiments. These experiments are planned to be focussed not only on the total and differential cross sections but also on the polarization of the scattered photons which might be even more sensitive to higher-order Coulomb corrections.

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- *j.sommerfeldt@tu-braunschweig.de
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