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On higher–order corrections to nuclear bremsstrahlung cross sections

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ABSTRACT

A quantitative understanding of bremsstrahlung by electrons in the screened field of atomic nuclei has been developed by several researchers over the last 80 years. However, some ranges of the possible parameters can still not be covered with good accuracy. Dirac partial-wave calculations are the best method developed to date, while analytic calculations are the only viable solution at high impinging electron energies. Recent progresses on both fronts will be discussed. In particular, state of the art partial wave results, including screening, allowed to test the Olsen–Maximon–Wergeland additivity rule discovered by analytic means. Closed expressions for the next-to-leading order corrections to the Furry–Sommerfeld–Maue wave functions are known. One next-to-next-to-leading order term is typically included in this type of approach. The effect of this extra term on the angular dependence of the double differential cross sections for photon emission by 2.5 MeV electrons is compared in detail with partial wave calculations which are exact at all orders.

1. Introduction

The basic description of bremsstrahlung emission by an electron in the Coulomb field of the atomic nucleus is known since more than 80 years ago, when the first non-relativistic calculation by Sommerfeld (1931) and the first relativistic ones by Sauter (1934), Bethe and Heitler (1934), Bethe (1934), and Racah (1934) were performed within the first Born approximation. Bethe and Maximon (1954) discovered that such a method is too crude for a process happening in a Coulomb field by employing the Furry–Sommerfeld–Maue (FSM) wave functions (Furry, 1934; Sommerfeld and Maue, 1935). They found that non-vanishing corrections remain present even in the high energy limit. The difficulties exposed by Bethe and Maximon have only been removed with partial success over the following 60 years: they stem from two main origins: i) the exact solution of the Dirac equation, even for a pure point-like Coulomb field, is not known in closed analytic form and ii) the field of the atomic nucleus is screened by the presence of the atomic electrons and this has to be included in the calculations. A full solution to both issues, that can be employed for all atomic numbers, impinging electron energies, and photon emission angles is still missing nowadays.

Two main routes of approach to these difficulties have been followed along the years: one heavily numeric based on the expansion of the initial and final electron wave functions in terms of partial waves and one analytic trying to include higher-order corrections to the FSM wave functions. A review of the latter was published recently by Mangiarotti and Martins (2017). Here we will discuss further progress made on both fronts.

2. Dirac partial-wave calculations

This method is based on partial wave expansions of the initial and final electron wave functions, that are then inserted into the Fermi Golden Rule to obtain a triple differential cross section (TDCS). By representing the photon field as a superposition of angular momentum eigenstates, the angular integrals (i.e. the one over all directions in space, appearing in the Fermi Golden Rule, and the one over the solid angle of the final electron necessary to arrive at a double differential cross section (DDCS)) can be evaluated analytically, leaving only radial ones to be performed numerically (see e.g. the paper by Tseng and Pratt (1971)). Because the continuum wave functions occurring in such integrals oscillate strongly, this step is the most serious difficulty that has to be overcome to obtain reliable values of the cross section. The first calculations with this Dirac partial-wave (DW) method were performed by Tseng and Pratt (1971), who were able to produce an extensive set of tables covering all elements and impinging electron energies E_e up to 2 MeV (Pratt et al., 1977, 1981). The main advantage of this approach was already exploited by Tseng and Pratt: since the radial integrals have anyhow to be performed numerically, the partial wave expansion can be applied to realistic (numerical) wave functions for a radially symmetric potential which includes the screening by the atomic electrons (described accurately with the help of atomic structure calculations). However, in order to advance to higher values of E_e, the number of partial waves necessary for convergence increases dramatically. This makes the computation extremely time-consuming. Only sparse attempts were made by Tseng and Pratt (1979) to reach energies above 2 MeV up to 10 MeV.

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An important progress over the work by Tseng and Pratt was made by Yerokhin and Surzhykov (2010), who borrowed the complex-plane rotation method (CRM) from nuclear physics to cope with the strongly oscillating radial integrals of bremsstrahlung. This improves the quality and stability of the results, but it is important to note that it does not reduce the number of partial waves needed to achieve convergence for a certain value of E_e. Moreover, in particular at backward angles and with increasing E_e, the TDCS starts to oscillate with the number of partial waves which are included in the calculation. Yerokhin and Surzhykov published results up to $E_e = 3$ MeV. Jakubassa-Amundsen (2016) extended the CRM to cover the case of nuclear finite-size potentials. Refining the numerical code, it became possible to cover energies up to $E_e = 30$ MeV for some selected geometries.

Mangiarotti and Jakubassa-Amundsen (2017) have noted recently that the code by Jakubassa-Amundsen can be coupled with the Olsen–Maximon–Wergeland (OMW) additivity rule (Olsen et al., 1957), known analytically, to include screening in an exact calculation for a pure nuclear field. The main advantage being that, for a potential that is Coulomb-like at large distances, the solution of the Dirac equation for scattering states possesses an asymptotic representation in terms of Whittaker functions (Yerokhin and Surzhykov, 2010), allowing to speed up the convergence of the radial integrals. The OMW prescription stipulates that, at high energies, it is possible to determine the exact cross section with screening by correcting the exact cross section without screening by the difference between screening and no screening obtained in the first Born approximation

$$\left(\frac{d^2\sigma}{dk\, d\Omega_k}\right)^{\text{screened}}_{\text{exact}} \approx \left(\frac{d^2\sigma}{dk\, d\Omega_k}\right)^{\text{no screening}}_{\text{exact}} + \left[\left(\frac{d^2\sigma}{dk\, d\Omega_k}\right)^{\text{screened}}_{\text{Born}} - \left(\frac{d^2\sigma}{dk\, d\Omega_k}\right)^{\text{no screening}}_{\text{Born}}\right], \quad (1)$$

where k is the momentum of the photon and $d\Omega_k$ its solid angle of emission. It is important to remark, as noted by Olsen (1955), that such an additivity rule can only be applied to single or double differential cross sections but not to triple differential cross sections.

The use of Eq. (1) was validated by Mangiarotti and Jakubassa-Amundsen (2017) employing DW calculations with screening from Tseng and Pratt (1971). However, by using a realistic atomic potential in the Salvat et al. (1995) code RADIAL for solving the Dirac equation, and employing the Yerokhin and Surzhykov prescription of the CRM for neutral potentials, it is possible to directly check the applicability of Eq. (1), as done in Fig. 1. The red squares are the results for the DDCS from a DW calculation for a pure point-like Coulomb field. The red dot-dashed line is obtained by interpolating these points with a spline and including screening via Eq. (1) using the first Born approximation and the atomic form factors by Hubbell et al. (1975, 1977). The blue solid line is the spline interpolation to the DW calculations for a realistic central potential (which takes into account finite nuclear sizes, even if they are irrelevant for the calculations presented). The two lines are very close, indicating the validity of the OMW additivity rule. The other two curves in Fig. 1 represent analytic approaches and are discussed in the next section. The agreement with the experimental data, for the case shown here in Fig. 1 and the others shown in the paper by Mangiarotti and Jakubassa-Amundsen (2017), demonstrates that, for E_e above 1 MeV and within current experimental accuracies, the inclusion of higher-order corrections to the initial and final electron wave functions, is, in principle, only necessary for the evaluation of the cross section in a pure point-like Coulomb field, while the effect of screening can be calculated to leading order within the first Born approximation.

For a small photon energy with respect to E_e, where screening effects are large, we have investigated the accuracy of the OMW additivity rule for even smaller collision energies. As shown in Fig. 2, the results from the screened DW calculations and from the OMW-corrected unscreened DW calculations are in fairly good agreement, except at the lowest energies. The differences are larger for Pb than for Sn, under the

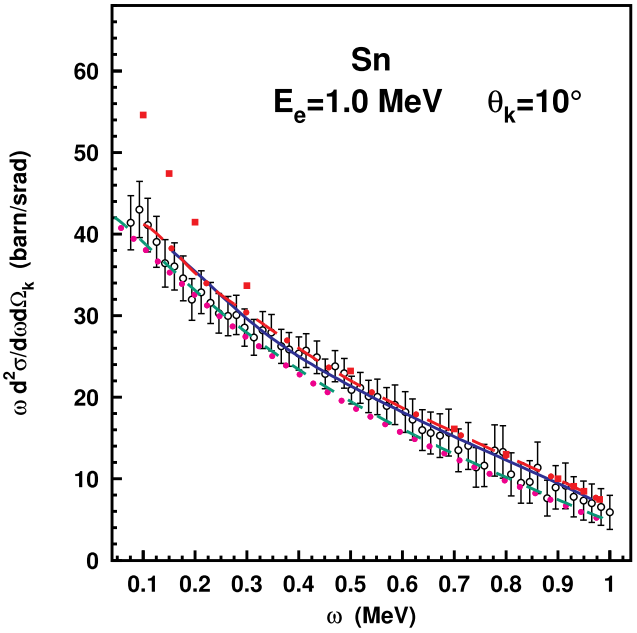

Fig. 1. Bremsstrahlung DDCS for 1.0 MeV electrons colliding with Sn and emitting photons at an angle of $\vartheta_k = 10°$ as a function of the photon energy ω. Legend: filled squares (red), unscreened DW; ——— (blue), screened DW; −·−·− (red), OMW-corrected unscreened DW; ····· (pink), screened LO; − − − − − (green), screened NNLO; circles with error bars, experiment (Rester and Dance, 1967). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

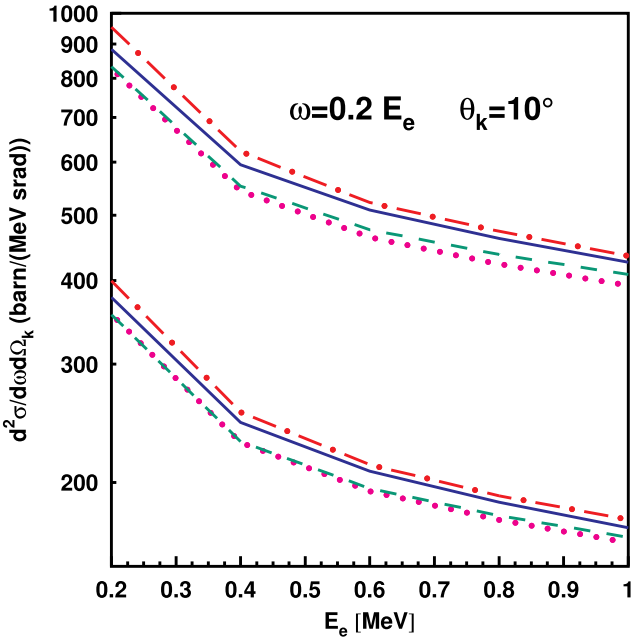

Fig. 2. Bremsstrahlung DDCS for electrons colliding with Sn and Pb as a function of the kinetic energy E_e of the impinging electron for a photon emission angle of $\vartheta_k = 10°$ and a photon energy $\omega = 0.2\, E_e$. Upper curves, Pb; lower curves, Sn. Legend: ——— (blue), screened DW; −·−·− (red), OMW-corrected unscreened DW; ····· (pink), screened LO; − − − − − (green), screened NNLO. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

same conditions.

3. Analytic calculations

The Dirac equation, which is a linear first–order partial differential equation (PDE), can be transformed into the iterated Dirac equation, which is a linear second–order PDE, as suggested by Sommerfeld and Maue (1935). The iterated Dirac equation, when only the terms of leading order in $\alpha\, Z$ are kept (where α is the fine structure constant and Z the nuclear charge), has the same structure as the Schrödinger equation and can thus be solved exactly for a pure point-like Coulomb field. The electron wave function in a pure point-like Coulomb field can then be written as

$$\Psi = \psi_0 + (\alpha\, Z)\, \psi_1 + (\alpha\, Z)^2\, \psi_2 \; + \; \cdots, \tag{2}$$

where the expansion point ψ_0 is the mentioned exact solution of the iterated Dirac equation to leading order. Sommerfeld and Maue also obtained a closed form for the next-to-leading order (NLO) correction to the wave function (for consistency, NLO terms have also to be added to the iterated Dirac equation) arriving at the following approximation of the initial and final electron wave functions

$$\Psi_{\mathrm{FSM}} \; = \; \psi_{\mathrm{a}} \; + \; \psi_{\mathrm{b}}, \tag{3}$$

where $\psi_{\mathrm{a}} = \psi_0$ and $\psi_{\mathrm{b}} = (\alpha\, Z)\, \psi_1$. The form suggested earlier by Furry (1934) is actually less friendly to be manipulated than the one found by Sommerfeld and Maue.

Because ψ_{a} already contains part of the interaction in a nonlinear way, establishing a fixed order in $\alpha\, Z$ of the nuclear bremsstrahlung matrix elements generated by Ψ_{FSM} is not trivial. However, as proved by Bethe and Maximon (1954), all the matrix elements of first order in $\alpha\, Z$ are considered in

$$M_{\mathrm{BM}} \; = \; M_{\mathrm{2a,1a}} \; + \; M_{\mathrm{2a,1b}} \; + \; M_{\mathrm{2b,1a}}, \tag{4}$$

where the subscripts indicate whether ψ_{a}, subscript (a), or ψ_{b}, subscript (b), are used for the initial, subscript (1), or final, subscript (2), states. Elwert and Haug (1969) performed the first complete calculation of the TDCS without any further approximation, beyond the use of the matrix elements from Eq. (4).

Higher order corrections in the framework of the FSM wave functions were considered by Roche et al. (1972) (a review of the attempts to include higher-order corrections in the framework of the Born approximation was given by Mangiarotti and Martins (2017)). The difficulties that have to be overcome are twofold. Firstly, the term of second order in $\alpha\, Z$ in the expansion of Eq. (2) has no closed analytic form. Roche et al. (1972) used an expression valid only in the high-energy limit and thus adopted for the initial and final electron wave functions the approximation

$$\Psi_{\mathrm{RDP}} = \Psi_{\mathrm{FSM}} + \psi_{\mathrm{c}} = \psi_{\mathrm{a}} + \psi_{\mathrm{b}} + \psi_{\mathrm{c}}\,, \tag{5}$$

where $\psi_{\mathrm{c}} = (\alpha\, Z)^2\, \psi_2$. Secondly, the result by Bethe and Maximon (1954) must be extended to establish all the matrix elements that have to be included to get a correct result for the TDCS at the NLO. This is not a trivial problem because it involves two degrees of freedom: one is $\alpha\, Z$ and the other is the electron energy. In fact, because of the initial approximation made in ψ_{c}, which can not be used at low energies, it does not make sense to include matrix elements of the correct NLO order in $\alpha\, Z$ which are unimportant in the high energy limit. Roche et al. (1972) investigated this question and found that all the NLO matrix elements relevant at high energies are

$$M_{\mathrm{RDP}} = M_{\mathrm{BM}} + M_{\mathrm{c}} \tag{6a}$$

$$M_{\mathrm{c}} = M_{\mathrm{2a,1c}} + M_{\mathrm{2c,1a}} \tag{6b}$$

and so, for example, the term $M_{\mathrm{2b,1b}}$ discarded by Bethe and Maximon (1954), compare Eqs. (4) and (6), continues to be omitted. Finally, one last issue is present when the square modulus of Eq. (6a) is taken. The consistent result at the NLO is

$$|M_{\mathrm{RDP}}|^2_{\mathrm{NLO}} = |M_{\mathrm{BM}}|^2 \; + \; 2\, \mathrm{Re}(M^{\star}_{\mathrm{BM}}\, M_{\mathrm{c}}) \tag{7}$$

However, Roche et al. (1972) maintained an extra next-to-next-to-leading order (NNLO) term originating from the square modulus of Eq. (6a),

$$|M_{\mathrm{RDP}}|^2_{\mathrm{NNLO}} = |M_{\mathrm{BM}}|^2 \; + \; 2\, \mathrm{Re}(M^{\star}_{\mathrm{BM}}\, M_{\mathrm{c}}) \; + \; |M_{\mathrm{c}}|^2 \tag{8}$$

because they argue that it can be easily calculated and it improves the agreement with low-energy data. This choice, to the best of our knowledge, has since then been followed by all authors who employed their results: Haug (2008), Mangiarotti and Martins (2016), Mangiarotti and Martins (2017) and Mangiarotti and Jakubassa-Amundsen (2017). However, it has to be clearly stressed that while Eq. (7) is a consistent truncation scheme of the expansion of the TDCS in $\alpha\, Z$ at high energies, since it includes all terms at the NLO important at high energies, Eq. (8) is not a consistent expansion of the TDCS in $\alpha\, Z$ at high energies because other NNLO terms of the same order and most probably important at high energies are missing. The actual formulae for the TDCS can be found in the mentioned references (Roche et al., 1972; Haug, 2008; Mangiarotti and Martins, 2016, 2017).

To compare this kind of calculations with data, one last step is missing: the inclusion of screening, which is accomplished along the lines described in the previous section employing the OMW additivity rule, i.e. Eq. (1). This was actually suggested by Haug (2008) and then has been employed to study the high-energy limit by Mangiarotti and Martins (2016). The arguments given by Mangiarotti and Jakubassa-Amundsen (2017) and strengthened in the previous section, justify this approach for electron energies near and above $\approx$ 0.5–1 MeV. Generally, the measurements of DDCSs are well reproduced for low–Z elements at all photon energies and also for intermediate–Z ones, if not too large angles are involved (see Fig. 1 and the results presented in our earlier works). For high–Z elements, a specific failure has been identified at large angles or close to the high energy limit, even for small angles. As shown by Mangiarotti and Jakubassa-Amundsen (2017), these deficiencies are not present when the OMW additivity rule is applied to the exact unscreened cross sections from the DW method and are hence not due to the use of such a rule, but rather to the adoption of inconsistent analytic calculations for the unscreened cross sections.

Here we want to investigate how much of this failure, in particular for the DDCS at increasing photon emission angles, is due to the use of just one NNLO extra term in Eq. (8). To this aim, we compare systematically the DDCSs obtained from Eq. (7) with the ones from Eq. (8) for Cu at 2.5 MeV in Fig. 3. When experimental data are missing, we use as reference for the correct results the DW calculations obtained with the use of the unscreened DDCSs for a pure point-like Coulomb field (finite nuclear size effects are absent for Cu even at 2.5 MeV and for a photon emission angle of 150°) and the OMW additivity rule. It is clear that the LO calculations underestimate, at large angles, the DW results, correct at all orders, while including the NLO terms consistently brings a rather good agreement. Contrary to the previously widespread belief, the NNLO term results in an overestimation of the cross section that increases with angle. This problem was noticed already by Mangiarotti and Jakubassa-Amundsen (2017), but there the adverse effect of this single NNLO term was not sorted out separately from all the others. As shown in that paper, the agreement for Al is already good at the LO for all angles, here we have shown that when the NLO correction is applied, Cu is also rather well reproduced. By comparing the red squares, that are the DDCSs from a DW calculation for a pure point-like Coulomb field, with the red solid curves, that are the corresponding DDCSs for the atomic potential obtained by a spline interpolation and the OMW additivity rule, it can be concluded that screening is irrelevant in all cases except for Fig. 3a and below $\approx$ 1.25 MeV. Thus, only the analytic calculation for a pure point-like Coulomb field can be responsible for the mentioned behaviour at large angles. It is possible to grasp

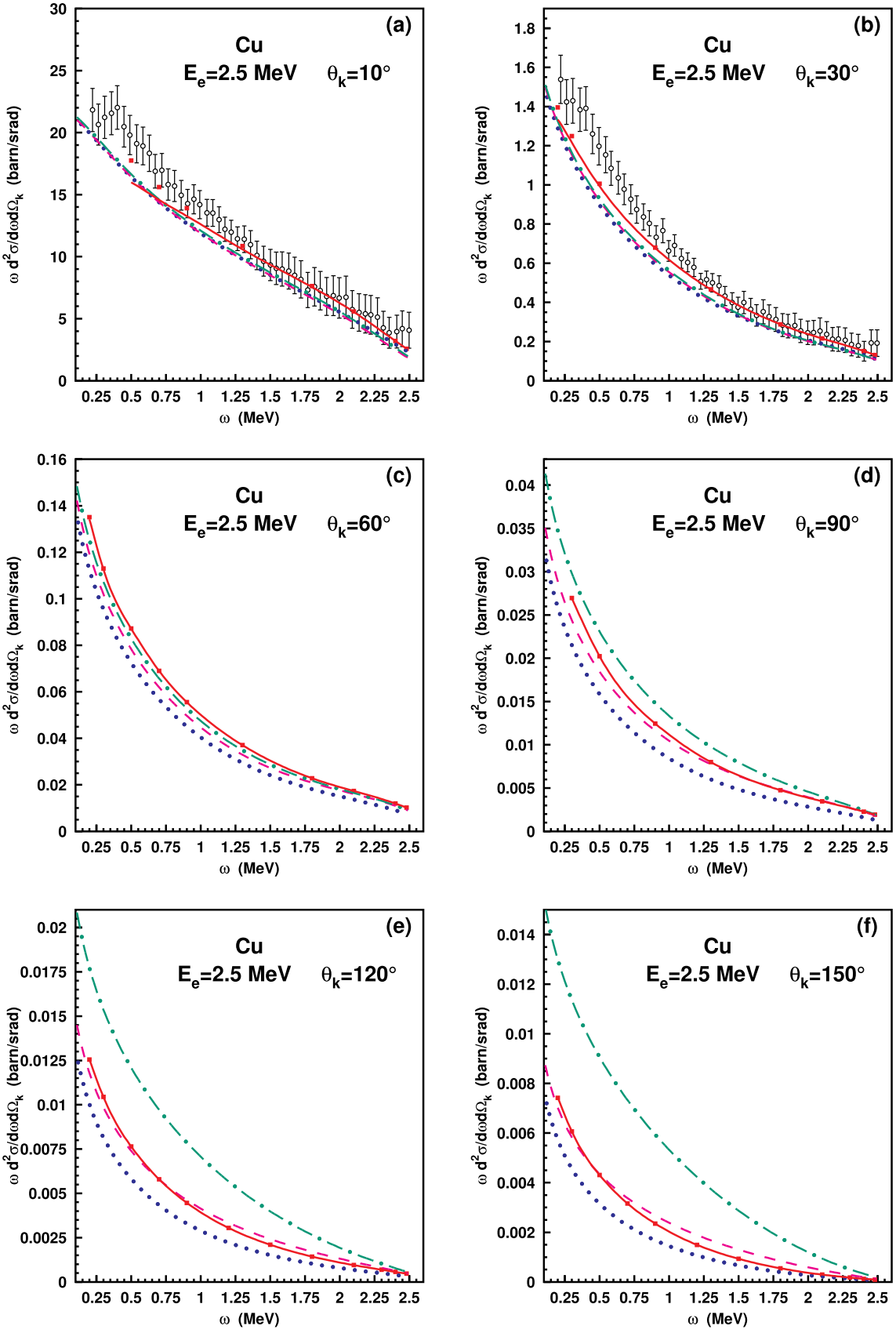

Fig. 3. Bremsstrahlung DDCS for 2.5 MeV electrons colliding with Cu at photon emission angles of (a) 10°, (b) 30°, (c) 60°, (d) 90°, (e) 120°, and (f) 150° as a function of the photon energy ω. Legend: filled squares (red), unscreened DW; ——— (red), OMW-corrected unscreened DW; ····· (blue), screened LO; – – – – – (pink), screened NLO; –·–·– (green), screened NNLO; circles with error bars, experiment (Rester and Dance, 1967).

intuitively that both the NLO correction is more important at larger angles and that screening is absent, because under such a condition the momentum transfer is higher and semi-classically the photon is emitted closer to the nucleus, where the initial and final electrons are poorly approximated by a plane wave or the FSM expression and the effect of the atomic electrons is small.

4. Conclusions

Current analytic models for bremsstrahlung double differential cross sections have been tested by a comparison with the state-of-the-art Dirac partial-wave theory. In particular, it has been found that the OMW additivity rule, combined with the DW theory for unscreened targets, gives very good results for collision energies above $\approx$ 0.5–1 MeV, which proves the applicability of this prescription when screening has to be taken into account. Moreover, it has been shown that the distortion effects of the initial and final electron wave functions close to the nucleus are reasonably well reproduced at all photon energies and angles by the NLO prescription, for atomic numbers approximately up to that of Cu, while the use of just one NNLO term, as conventionally done in analytic bremsstrahlung models, leads to incorrect results at the higher angles.

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