On the stripping approximation in the bremsstrahlung process

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Abstract. We discuss two different approaches for the approximate treatment of the bremsstrahlung (BrS) process of non-relativistic electrons on many-electron atomic/ionic targets, described by a total amplitude which is a sum of ordinary and polarizational BrS amplitudes. The approaches are based on the so-called 'stripping' effect; they are useful for calculation of the BrS spectra for photon energies greater than the outer shell thresholds.

1. Introduction.

The aim of this paper is to present a consistent comparison of two different approaches proposed recently (Korol *et al* 1999, and Avdonina and Pratt 1999) for an approximate treatment of the bremsstrahlung process of non-relativistic electrons on many-electron atomic/ionic targets. Both approaches are based on the so-called 'stripping' effect, which says that with increasing photon energy ω the decrease of ordinary bremsstrahlung due to screening is partly (or completely in the Born approximation) compensated by the additional polarizational radiation. A 'stripping' approximation, based on this effect, is efficient for obtaining BrS spectra for photon energies greater than the ionization thresholds of the atom/ion. There are two main accomplishments. (1) In this paper we give a more complete presentation, as well as more systematic numerical results, of the approach of Korol *et al* 1999. (2) The comparison of the results of the two approaches

allows us to better justify the applicability of the approximation proposed by Avdonina and Pratt (1999). In this paper the atomic system of units will be used.

The term 'stripping' effect and the original idea are due to Amusia *et al* (1985), where the BrS process was considered within the framework of the non-relativistic Born approximation and for the dipole-photon range. Within these approximations stripping had previously been demonstrated for the special case of hydrogen for $\omega \gg I_{1s}$ (Buimistrov and Trakhtenberg 1975), where the BrS cross section reduces to the spectrum of the bare nucleus. The shell-by-shell 'stripping' effect was then demonstrated by results of numerical calculations of BrS of fast electrons obtained in the Born approximation (Amusia *et al* 1986, Avdonina *et al* 1986). For the sake of clarity we reproduce the arguments describing the 'stripping' effect.

The BrS emission during a collision of a fast but non-relativistic electron with a many-electron atom (ion) arises due to (i) acceleration of the projectile in the static field of the target (ordinary BrS), and due to (ii) the virtual polarization of target electrons under the action of the field of the projectile, - the polarizational BrS (Amusia *et al* 1976, 1977, 1982, Buimistrov and Trakhtenberg 1975,1977, Zon 1977, 1979, Wendin and Nuroh 1977, Pindzola M S and Kelly 1976). Both types of BrS radiation have been considered later in various connections (see the reviews of Amusia 1988, Amusia and Pratt 1992, Korol and Solov'yov 1997, and references therein).

Considering the two mechanisms of photon emission, and utilizing the Born approximation, one evaluates the following expression for the total amplitude of the process:

$$f_{\rm tot} = f_{\rm ord} + f_{\rm pol} = \frac{4\pi(\mathbf{e}\cdot\mathbf{q})}{q^2}\left[\frac{Z-F(q)}{\omega} - \omega\,\alpha(\omega,q)\right], \qquad (1)$$

where $\mathbf{e}$ and ω are the photon polarization vector and energy, $\mathbf{q}$ is the transferred momentum, Z is the atomic number, and $F(q)$ is the atomic electron form-factor. As $q \longrightarrow 0$ $F(q)$ reduces to the total number of target electrons N ($N = Z$ for a neutral atom).

The first term in (1), proportional to $Z - F(q)$, describes the ordinary part of the BrS amplitude. The polarizational part, the second term in (1), is expressed via a so-called generalized atomic polarizability. This function is defined so that it reduces to the dipole dynamic polarizability, $\alpha(\omega)$, in the limit of small transferred momenta, $\lim\limits_{q\to 0}\alpha(\omega,q) = \alpha(\omega)$.

The ω dependence of $\alpha(\omega,q)$ reflects the ability of the cloud of atomic electrons to be dynamically polarized by an external electromagnetic field of a given frequency. In a many-electron atom the electrons are distributed among the atomic subshells. Each subshell is characterized by an ionization potential I. In terms of classical mechanics the quantity I corresponds to the frequency of the rotation of electrons of a given subshell

around the nucleus. Using this analogy one may say that the dynamic response of the electron cloud to the external field will increase for those ω which are close to the ionization thresholds of the target subshells. Therefore, in the region

$$I_1 \leq \omega \leq I_{1s} \tag{2}$$

where I_1 and I_{1s} stand, respectively, for the ionization potentials of the outer shell and of the $1s$ shell, the behaviour of $\alpha(\omega, q)$ as a function of ω will be essentially non-monotonic with extrema in vicinities of the subshell ionization potentials.

In the region of high photon energies, $\omega \gg I_{1s}$,

$$\alpha(\omega, q) \approx -\frac{F(q)}{\omega^2}\,. \tag{3}$$

As a result the amplitude f_{tot} reduces to the BrS amplitude of the fast electron on a bare nucleus (Amusia *et al* 1985):

$$f_{tot} \approx \frac{4\pi(\mathbf{e}\cdot\mathbf{q})}{q^2}\,\frac{Z}{\omega}\,. \tag{4}$$

This shows that in the region of large photon energies the atomic electron do not participate in the screening of a nucleus and do not contribute to the BrS cross section.

The physical reason for this de-screening (or 'stripping') effect is that, for $\omega \gg I_{1s}$, the electrons of all atomic subshells may be treated as free. Then, if the incident electron is also free (the Born approximation), there is no dipole radiation in a system of free electrons, since it possesses no accelerating dipole moment.

This effect can also be explained in terms of the interference between ordinary and polarizational BrS which, being constructive in the region of high photon frequencies, leads to an increase in the cross section for total BrS.

These arguments allow one to construct (still operating within the Born approximation) an approximate expression for the total BrS amplitude also for photon energies lower than the K-shell ionization threshold (Amusia *et al* 1985). In a many-electron target, where the threshold potentials of different subshells are well separated, the electrons can be divided into two groups, the 'inner' and the 'outer' electrons, with respect to the photon energy. The inner electrons are those whose binding energies, I_{in}, exceeds ω. Correspondingly, the outer electrons have the binding energies I_{out} less than ω:

$$I_{out} < \omega < I_{in}\,. \tag{5}$$

The cloud of inner electrons is not distorted (polarized) noticeably by an external electromagnetic field of such a frequency ω and, thus, these electrons do not contribute to the amplitude of the polarizational BrS. On the other hand, the outer electrons behave as free under the action of the field, and their contribution to f_{pol} can be described

by eq. (3) where one substitutes the quantity $F(q)$ with the form-factor of the outer electrons only, $F_{\rm out}(q)$. As a result the total BrS amplitude acquires the form

$$f_{\rm tot} \approx \frac{4\pi(\mathbf{e}\cdot\mathbf{q})}{q^2}\left[\frac{Z-F(q)}{\omega}+\frac{F_{\rm out}(q)}{\omega}\right]=\frac{4\pi(\mathbf{e}\cdot\mathbf{q})}{q^2}\,\frac{Z-F_{\rm in}(q)}{\omega}\,, \qquad (6)$$

where $F_{\rm in}(q)$ stands for the form-factor of the inner electrons. The expression on the right-hand side clearly demonstrates that the outer electrons do not participate in the screening of the nucleus (or, in other words, the nucleus is 'stripped' by a total number $N_{\rm out}$ of the outer electrons). The physical reason for this partial 'stripping' is as formulated above: for $\omega > I_{\rm out}$ the outer electrons can be considered as free and, therefore, there is no dipole-photon emission by the system 'projectile electron + the outer electrons'.

On the basis of these considerations one draws the following qualitative picture of the behaviour of the total BrS cross section as a function of emitted photon energy. Let a target have n subshells which are labeled with $j = 1 \ldots n$ ($j = 1$ corresponds to the outermost subshell, $j = n$ stands for the 1s-shell). The number of electrons in each subshell is N_j. In the region $\omega < I_1$, where all electrons could be considered as inner and, thus, do not contribute to the polarizational part of the amplitude, the total BrS cross section σ is equal to σ_0, which is the ordinary BrS cross section for the given atomic/ionic target. As ω increases then more electrons belong to the outer group leading to an effective decrease in the screening of the nuclear field. Within the range $I_j < \omega < I_{j+1}$ the dependence $\sigma(\omega)$ follows the smooth pattern of the ordinary BrS cross section in the Coulombic field of a charge $Z - \sum_{i=j+1}^{n} N_j$. At the threshold of the j-th subshell the cross section $\sigma(\omega)$ experiences a jump, the magnitude of which is proportional (approximately) to N_j^2. For $\omega > I_n \equiv I_{1\rm s}$, where all the electrons are treated as outer, the emission occurs as in the field of the bare nucleus.

This clear physical picture was initially derived (Amusia *et al* 1985) and confirmed by numerical calculations (Amusia *et al* 1986, Avdonina *et al* 1986) within the framework of the non-relativistic Born approximation. Later the stripping approximation was generalized, going beyond the Born approximation, for the case of intermediate energy projectile electrons. Using a partial wave approximation Korol (1992) established the 'stripping' effect for the high photon energy region $\omega \gg I_{1\rm s}$. In this limit only the nuclear field contributes effectively to the total BrS (6).

In the work of Korol *et al* (1999) the approach of Korol (1992) beyond Born approximation was generalized to describe the case of all possible photon energies in the non-relativistic region of the projectile energies. The results of calculations of BrS spectra of 25 keV electrons from Ar and Ne obtained in the framework of this 'stripping' approach were presented, to compare with the results of the partial wave approximation.

To simplify the complex problem of the exact evaluation of the total BrS spectra from atoms and ions at non-Born projectile energies, a 'stripping' approach was also

developed by Avdonina and Pratt (1999), directly applying the result of the 'stripping' approximation to the region of low relativistic energies where Born approximation was not valid. The advantage of this approach is that it reduces direct calculations of the BrS amplitude to the analysis of the free-free dipole photon matrix elements of ordinary BrS in a point Coulomb field, and in screened Coulomb potentials. For the ordinary BrS spectra from neutral atoms and positive ions, including the case of Coulombic BrS, a simple parametrization was developed by Avdonina and Pratt 1997a,b, 1999). Since the accuracy achieved by applying the parametrization is fairly good in a wide range of projectile energies and radiation fraction (at least, it is not significantly worse than the accuracy of the partial wave calculations), these expressions can be successfully used for calculation of the total BrS spectra within the corresponding ranges of photon energies $I_j < \omega < I_{j+1}$, as described above. Note, however, that the parametrization was not applicable either for relativistic incident electron energies or for energies smaller than 10 keV.

In this paper we will give more results of both 'stripping' approaches and we will compare them with each other. Formally, both 'stripping' approaches [Avdonina and Pratt (1999) and Korol *et al* (1999)] result in similar-looking formulae for the principal part of the total BrS amplitude, expressing it in terms of a single-electron transition under the action of an effective acceleration operator which depends on the energy of the emitted photon (for details see sections 2 and 3). The major difference between the two approximate formulae, eqs. (20) and (25), is that they utilize different sets of initial/final state wavefunctions of the projectile. In (20), which is based on the approach due to Korol (1992), the projectile wavefunctions are obtained as solutions of the Schrödinger equation with the potential created by the target nucleus and by *all* of its electrons. The method of Avdonina and Pratt (1999), eq. (25), implies that the potential, entering the Schrödinger equation, is dependent on the photon energy. Namely, for ω satisfying (5) the potential consists of the nuclear part and of a part due to the inner electrons only.

Although both approximate formulae reduce to eq. (6) in the Born limit, it is unclear to what extent they coincide/deviate if one considers different targets, incident electron energies and ranges of ω. It is the aim of this paper to carry out this comparison. To do this we have computed the BrS spectra over a wide range of photon energies and for various projectile energies and atomic targets. The results are presented in section 4.

To conclude the introductory part we mention that both approaches, as well as the 'stripping' approximation itself, become inadequate for relativistic projectiles, where the effects of retardation (see Amusia *et al* (1985) and Astapenko *et al* (1985)), and the radiation of higher multipoles strongly influence the BrS spectrum. However, in this case it is possible to represent the BrS total amplitude in terms of the free-free matrix element of some effective operator (Korol *et al* 2001).

2. The 'stripping' effect beyond the Born approximation

In this section we demonstrate how the 'stripping' approximation formulated in section 1 can be generalized to the case of a non-Born projectile.

Assuming the energies of the projectile electron before (ε_1) and after (ε_2) the collision to be high enough compared to the energies of the target electrons, one can neglect exchange effects and consider the motion of the projectile in the atomic (ionic) frozen-core potential

$$V_{\rm at}(\mathbf{r}) = -\frac{Z}{r} + V_0(\mathbf{r})\,. \tag{7}$$

The first term is the Coulomb potential of the atomic nucleus, the second is the potential created by the atomic electron cloud:

$$V_0(\mathbf{r}) = \int \mathrm{d}\mathbf{r}_1 \ldots \mathrm{d}\mathbf{r}_N \sum_{a=1}^{N} \frac{|\psi_0(\{\mathbf{r}_a\})|^2}{|\mathbf{r}-\mathbf{r}_a|}\,. \tag{8}$$

The sum is carried out over all atomic electrons. The notation $\mathbf{r}_a$ stands for the radius vector of the a-th electron, the quantity $\psi_0(\{\mathbf{r}_a\})$ is the ground state atomic wavefunction dependent on the radius vectors of all electrons, $\{\mathbf{r}_a\} \equiv \mathbf{r}_1 \ldots \mathbf{r}_N$.

The projectile wavefunctions of the initial, $\psi^{(+)}_{\mathbf{p}_1}(\mathbf{r})$, and the final, $\psi^{(-)}_{\mathbf{p}_2}(\mathbf{r})$, states satisfy the equation

$$\left[\frac{\hat{p}^2}{2} + V_{\rm at}(\mathbf{r})\right]\psi^{(\pm)}_{\mathbf{p}}(\mathbf{r}) = \varepsilon\,\psi^{(\pm)}_{\mathbf{p}}(\mathbf{r})\,. \tag{9}$$

The superscripts plus and minus correspond to the outgoing ('+') and the incoming ('-') boundary conditions imposed on the asymptotic behaviour of the wavefunctions.

In the lowest order of the non-relativistic perturbation theory in the electron—dipole-photon interaction and in the interaction, between the projectile and the atomic electrons,

$$\hat{V} \equiv \hat{V}(\mathbf{r},\{\mathbf{r}_a\}) = \sum_{a=1}^{N} \hat{v}^{(a)}, \qquad \hat{v}^{(a)} = \frac{1}{|\mathbf{r}-\mathbf{r}_a|}\,, \tag{10}$$

which leads to virtual atomic excitations, the amplitudes $f_{\rm ord}$ and $f_{\rm pol}$ are written as follows:

$$f_{\rm ord} = \langle \mathbf{p}_2^{(-)}\,|\mathbf{e}\cdot\hat{\mathbf{p}}|\,\mathbf{p}_1^{(+)}\rangle\,, \tag{11}$$

$$f_{\rm pol} = -\sum_{a=1}^{N}\sum_{n}\left\{\frac{\langle 0|\mathbf{e}\cdot\hat{\mathbf{p}}_a|n\rangle\langle n|\hat{v}^{(a)}_{\mathbf{p}_2\mathbf{p}_1}|0\rangle}{\omega_{n0}-\omega-\mathrm{i}0} + \frac{\langle 0|\hat{v}^{(a)}_{\mathbf{p}_2\mathbf{p}_1}|n\rangle\langle n|\mathbf{e}\cdot\hat{\mathbf{p}}_a|0\rangle}{\omega_{n0}+\omega}\right\} \equiv f^{(\rm r)}_{\rm pol} + \mathrm{i}\,f^{(\rm i)}_{\rm pol}\,, \tag{12}$$

$$f^{(\rm r)}_{\rm pol} = -\sum_{a=1}^{N}\,\mathrm{v.p.}\sum_{n}\left\{\frac{\langle 0|\mathbf{e}\cdot\hat{\mathbf{p}}_a|n\rangle\langle n|\hat{v}^{(a)}_{\mathbf{p}_2\mathbf{p}_1}|0\rangle}{\omega_{n0}-\omega} + \frac{\langle 0|\hat{v}^{(a)}_{\mathbf{p}_2\mathbf{p}_1}|n\rangle\langle n|\mathbf{e}\cdot\hat{\mathbf{p}}_a|0\rangle}{\omega_{n0}+\omega}\right\}, \tag{13}$$

$$f^{(\rm i)}_{\rm pol} = -\pi\sum_{a=1}^{N}\sum_{n}\langle 0|\mathbf{e}\cdot\hat{\mathbf{p}}_a|n\rangle\langle n|\hat{v}^{(a)}_{\mathbf{p}_2\mathbf{p}_1}|0\rangle\,\delta(\omega_{n0}-\omega)\,. \tag{14}$$

Here '0' and 'n' denote the ground and excited states of the target, ω_{n0} is the transition energy, $\hat{\mathbf{p}}_a$ is the momentum operator of the a-th electron, $\hat{v}^{(a)}_{\mathbf{p}_2\mathbf{p}_1} = \langle \mathbf{p}_2^{(-)} | \hat{v}^{(a)} | \mathbf{p}_1^{(+)} \rangle$, and $\hat{\mathbf{p}}$ is the momentum operator of the projectile electron. The sum is carried out over all excited states including the excitations into the continuum.

The term $f^{(\mathrm{r})}_{\mathrm{pol}}$ (the real part of the polarizational amplitude) accounts for the virtual excitations $0 \longrightarrow n$.

The term $f^{(\mathrm{i})}_{\mathrm{pol}}$ (the imaginary part of the polarizational amplitude) describes a real two-step process: the excitation $0 \longrightarrow n$ under the action of the Coulomb interaction $\sum_{a=1}^{N} \hat{v}^{(a)}$ and the subsequent de-excitation accompanied by photon emission (the energy of the n state is fixed at $\varepsilon_n = \omega + \varepsilon_0$). This is constructed of two factors. The first factor, $\langle 0|\mathbf{e}\cdot\hat{\mathbf{p}}_a|n\rangle$, is proportional to the photoabsorption amplitude, while the second factor, $\langle n|\hat{v}^{(a)}_{\mathbf{p}_2\mathbf{p}_1}|0\rangle$, is related to the amplitude of atomic excitation (ionization) via electron impact.

To evaluate the limit of f_{pol} corresponding to the 'stripping' approximation one has to consider the transformation of $f^{(\mathrm{r})}_{\mathrm{pol}}$. For given ω, in accordance with (5), the atomic electrons are split into two groups, of inner and outer electrons. Assuming that the strong inequality $\omega \ll I_{\mathrm{in}}$ is fulfilled, one neglects the contribution of the virtual excitations of the inner electrons to the sum in (13). Then, the amplitude $f^{(\mathrm{r})}_{\mathrm{pol}}$ is defined by the contribution of the virtual excitations of the outer electrons:

$$f^{(\mathrm{r})}_{\mathrm{pol}} \approx -\sum_{a_{\mathrm{out}}} \mathrm{v.p.} \sum_n \left\{ \frac{\langle 0|\mathbf{e}\cdot\hat{\mathbf{p}}_{a_{\mathrm{out}}}|n\rangle\langle n|\hat{v}^{(a_{\mathrm{out}})}_{\mathbf{p}_2\mathbf{p}_1}|0\rangle}{\omega_{n0}-\omega} + \frac{\langle 0|\hat{v}^{(a_{\mathrm{out}})}_{\mathbf{p}_2\mathbf{p}_1}|n\rangle\langle n|\mathbf{e}\cdot\hat{\mathbf{p}}_{a_{\mathrm{out}}}|0\rangle}{\omega_{n0}+\omega} \right\}. \tag{15}$$

Using the inequality $\omega > I_{\mathrm{out}}$ one expands the denominators in powers of the small parameter ω_{n0}/ω: $(\omega_{n0} \pm \omega)^{-1} = \pm\omega^{-1} - \omega_{n0}\,\omega^{-2} + O(I_{\mathrm{out}}\omega^{-3})$. It can be demonstrated that the terms containing $\omega_{n0}\,\omega^{-2}$ do not contribute to the sum on the right-hand side of (15). The leading term, proportional to ω^{-1}, is evaluated with the help of the completeness relation $\sum_n |n\rangle\langle n| = 1$. The result is

$$f^{(\mathrm{r})}_{\mathrm{pol}} = \frac{\mathrm{i}\mathbf{e}}{\omega}\langle \mathbf{p}_2^{(-)} | \nabla_{\mathbf{r}} V_0^{(\mathrm{out})}(\mathbf{r}) | \mathbf{p}_1^{(+)} \rangle + O\left(\frac{I^2_{\mathrm{out}}}{\omega^3}\right), \tag{16}$$

where the quantity

$$V_0^{(\mathrm{out})}(\mathbf{r}) = \left\langle 0 \left| \sum_{a_{\mathrm{out}}} \frac{1}{|\mathbf{r}-\mathbf{r}_{a_{\mathrm{out}}}|} \right| 0 \right\rangle \tag{17}$$

is the part of the potential $V_0(\mathbf{r})$ (see eq. (8)) created by the outer electrons.

Therefore, the total amplitude of the BrS process (more exactly, its real part) can be represented as follows:

$$\mathrm{Re}\, f_{\mathrm{tot}} \approx \langle \mathbf{p}_2^{(-)} | \mathbf{e}\hat{\mathbf{p}} | \mathbf{p}_1^{(+)} \rangle + \frac{\mathrm{i}\mathbf{e}}{\omega}\langle \mathbf{p}_2^{(-)} \left| \nabla_{\mathbf{r}} V_0^{(\mathrm{out})}(\mathbf{r}) \right| \mathbf{p}_1^{(+)} \rangle . \tag{18}$$

To obtain the final expression for $f_{\rm tot}$ let us introduce the operator of the total acceleration $\hat{\mathbf{a}}_{\rm at}$ of the projectile in the field $V_{\rm at}(\mathbf{r})$ (see (7)):

$$\hat{\mathbf{a}}_{\rm at} = -\nabla_{\mathbf{r}} V_{\rm at}(\mathbf{r}) = -Z\,\frac{\mathbf{r}}{r^3} + \hat{\mathbf{a}}^{(\rm in)} + \hat{\mathbf{a}}^{(\rm out)}\,, \tag{19}$$

where $\hat{\mathbf{a}}^{(\rm out)}$ and $\hat{\mathbf{a}}^{(\rm in)}$ are the operators of the accelerations due to the potentials of the outer and the inner electrons.

Expressing the ordinary BrS amplitude (the first term in (18)) in terms of the matrix element of $\hat{\mathbf{a}}_{\rm at}$ one obtains the following expression for the total BrS amplitude within the 'stripping' approximation:

$$f_{\rm tot} \approx \frac{\rm i}{\omega}\langle \mathbf{p}_2^{(-)} \left| \mathbf{e}\cdot\hat{\mathbf{A}} \right| \mathbf{p}_1^{(+)}\rangle - {\rm i}\pi \sum_{a=1}^{N_{\rm out}} \sum_n \langle 0 \left| \mathbf{e}\cdot\hat{\mathbf{p}}_a \right| n\rangle \langle n \left| \hat{v}^{(a)}_{\mathbf{p}_2\mathbf{p}_1} \right| 0\rangle\, \delta\left(\omega_{n0} - \omega\right)\,. \tag{20}$$

The operator $\hat{\mathbf{A}}$ is defined as

$$\hat{\mathbf{A}} = -Z\,\frac{\mathbf{r}}{r^3} + \hat{\mathbf{a}}^{(\rm in)}\,. \tag{21}$$

The sum in the last term in (20) is carried out over the outer electrons. This is justified by the factor $\delta(\omega_{n0} - \omega)$ and the conditions (5).

Eq. (20) generalizes the result of Korol (1992), where the focus was on the high-frequency limit of the BrS spectrum, $\omega \gg I_{1\rm s}$, where all target electrons can be considered as 'inner' ones. The current scheme allows us to introduce the stripping effect for each atomic subshell by comparing its ionization potential with the photon energy.

Note that expression (20) is exact in the sense that in its derivation no approximate schemes have been used to describe the many-electron target. The result is applicable for any type of target (atomic, ionic, molecular).

Two assumptions, both of a general nature, are made to evaluate (20):

(i) the dynamics of the projectile is subject to the action of the frozen-core potential (see (7)) created by the target nucleus (or nuclei, if a many-atom molecule is considered) and electrons.

(ii) the process of photon emission (by both the projectile and the target) can be described within the frame of the dipole approximation.

The formula (20) establishes that for photon energies ω within the range defined by (5) the total BrS of an electron effectively consists of two terms.

The first term is a free-free transition matrix element of the operator $\hat{\mathbf{A}}$. The latter is defined in (21) and represents the effective acceleration of the projectile due to the action of the Coulomb field of the nucleus and the field of the inner-shell electrons. This matrix element has to be evaluated between the exact initial, $\psi^{(+)}_{\mathbf{p}_1}(\mathbf{r})$, and the final, $\psi^{(-)}_{\mathbf{p}_2}(\mathbf{r})$, projectile wavefunctions satisfying the Schrödinger equation (9) with the frozen-core potential (7). This term involves a joint action of the two mechanisms of

BrS formation: the ordinary one and the polarizational BrS, where only virtual atomic excitations are taken into account. The sum of these terms results, effectively, in the *renormalization of the vertex* describing the electron-photon interaction, but it leaves unchanged the projectile's wavefunctions.

The second term, $f_{\rm pol}^{\rm (i)}$, is due to the real excitations of the atom during the collision. This describes a two-step process which corresponds to the excitation of an outer-shell atomic electron under the action of the Coulomb interaction with the projectile and the subsequent radiative de-excitation. This term is of most importance for photon energies in vicinities of the outer-shell ionization thresholds.

To conclude this section let us mention that the Born limit of (20) is rather straightforward. Indeed, substituting in the first term for the wavefunctions $\psi_{\mathbf{p}_1}^{(+)}(\mathbf{r})$ and $\psi_{\mathbf{p}_2}^{(-)}(\mathbf{r})$ the corresponding plane waves, one obtains the formula (6). The contribution of the real excitations to the total BrS amplitude (the second term in (20)) was not accounted for when evaluating (6).

3. Alternative approach to the 'stripping' effect beyond the Born approximation

Different physical arguments were used by Avdonina and Pratt (1999) to formulate the 'stripping' approximation beyond the framework of the Born approximation for a projectile electron. Their approach can be summarized as follows.

Suppose that the photon energy lies between the ionization potential of two neighbouring atomic subshells,

$$I_{j-1} < \omega < I_j \,, \tag{22}$$

where $j = 1 \ldots n$ and n stands for the $1s$ subshell. In this case the Born formula (6) suggests that the total BrS process can be interpreted in terms of the radiative transition of an electron scattered by the field of a partly screened nucleus, $V_{\rm ion}(r) = -Z/r + V_{\rm in}(r)$, with $V_{\rm in}(r)$ being the potential due to the inner electrons only. As $r \longrightarrow \infty$ the potential $V_{\rm ion}(r)$ has the form of an ionic field with net charge $Z_{\rm ion} = Z - N_{\rm out}$, where $N_{\rm out} = \sum_{i=j+1}^{n} N_i$.

Let us extrapolate this clear physical picture (which is justified within the Born approximation) to the range of projectile energies where the Born approximation is not applicable to describe the scattering process. Thus, one assumes that within the 'stripping' approximation the real part of the total BrS amplitude can be expressed in terms of the matrix element

$$\mathrm{Re}\, \tilde{f}_{\rm tot} = \left\langle \tilde{\mathbf{p}}_2^{(-)} \,|\, \mathbf{e}\cdot\hat{\mathbf{p}} \,|\, \tilde{\mathbf{p}}_1^{(+)} \right\rangle \,, \tag{23}$$

where the tilde signs are written to distinguish between the quantities used here and the quantities introduce in the preceding section.

The wavefunctions $\tilde{\psi}_{\mathbf{p}}^{(\pm)}(\mathbf{r})$, which correspond to the scattering states $\left|\tilde{\mathbf{p}}^{(\pm)}\right\rangle$, satisfy the Schrödinger equation in the ionic field $V_{\rm ion}(r)$:

$$\left[\frac{\hat{p}^2}{2} + V_{\rm ion}(\mathbf{r})\right]\tilde{\psi}_{\mathbf{p}}^{(\pm)}(\mathbf{r}) = \varepsilon\,\tilde{\psi}_{\mathbf{p}}^{(\pm)}(\mathbf{r})\,. \tag{24}$$

Thus the calculation of the total BrS spectrum requires calculation of the spectrum of the neutral atom (for $\omega < I_1$) and for a number of ions (of the ionicities $Z - \sum_{i=j}^{n} N_i$, $j = 1 \ldots n$), as well as for the pure Coulomb spectrum (when $\omega > I_n \equiv I_{1\rm s}$). To obtain accurate data on BrS from neutral atoms for low relativistic energies of the projectile $1\,keV < \omega < 2000\,keV$ one can use tabulated results obtained in numerical relativistic partial-wave approximation (Pratt *et al* 1977a,b). Results for a few atomic ions, obtained in the similar way for a number of projectile energies and fraction of energy radiated were also available (Lee *et al* 1977). Recently simple analytic expressions for BrS spectra of atoms and their ions, including bare nuclei, for the energy range $10\,keV < \omega < 2000\,keV$ have been developed (Avdonina and Pratt 1997a,b,1999). The accuracy of these expressions is usually better than 5%, becoming worse with decreasing electron energy.

Despite the relative simplicity of its practical implementation, this approach is less justified from the formal viewpoint than the formulation of the 'stripping' approximation outlined in section 2. To indicate explicitly the difference between the matrix element (23) and its counterpart (20) let us reduce the matrix element of the momentum operator on the right-hand side of (23) to that of the acceleration operator. Then, taking into account equation (24) and recalling the definition (21), one notices that the operator $\hat{\mathbf{A}}$ is the total acceleration of the projectile in the field $V_{\rm ion}(\mathbf{r})$. Therefore

$$\mathrm{Re}\,\tilde{f}_{\rm tot} = \frac{\mathrm{i}}{\omega}\langle\tilde{\mathbf{p}}_2^{(-)}\left|\mathbf{e}\cdot\hat{\mathbf{A}}\right|\tilde{\mathbf{p}}_1^{(+)}\rangle\,. \tag{25}$$

Comparison of this result and the first term on the right-hand side of (20) illuminates the difference between the two approaches: both amplitudes are the matrix elements of the same operator $\hat{\mathbf{A}}$ but calculated using different initial/final state wavefunctions. In (20) the wavefunctions $\psi_{\mathbf{p}}^{(\pm)}(\mathbf{r})$ are the solutions of the Schrödinger equation (9) with the static potential (7) due to the target's nucleus and *all* electrons, whereas the wavefunctions $\tilde{\psi}_{\mathbf{p}}^{(\pm)}(\mathbf{r})$ are obtained from (24), where the potential $V_{\rm ion}(\mathbf{r})$ depends (implicitly) on the photon energy. Indeed, for $\omega > I_n = I_{1s}$ this potential reduces to the point Coulomb field $-Z/r$, for $\omega < I_1$ (no outer electrons) $V_{\rm ion}(\mathbf{r})$ coincides with (7), and for $I_1 < \omega < I_n$ the potential is given by $V_{\rm ion}(r) = -Z/r + V_{\rm in}(r) = V_{\rm at}(\mathbf{r}) - V_{\rm out}(r)$.

Prior to making a quantitative comparison of the two approaches to the 'stripping' approximation, let us point out the cases in which both treatments produce identical results. The first is the region of photon energies below the ionization threshold of the target. In this case (20) and the first term on the right-hand side of (20) coincide, since $V_{\rm ion}(\mathbf{r}) = V_{\rm at}(\mathbf{r})$. The second is the region of high photon energies, $\omega \gg I_{1\rm s}$, where

the amplitude $f_{\rm tot}$ reduces to the BrS amplitude of the fast electron on a bare nucleus. Finally, both approaches give identical results in the Born limit. Both formulae reduce to (6) if the scattering states are described by plane waves.

4. Numerical results

In this section we present the results of numerical calculations of the BrS spectra formed in the collision of an electron with $\varepsilon = 5 \ldots 50$ keV electron with neutral Ar, Kr, Xe, Au atoms ($Z = 18, 36, 54, 79$, correspondingly). The data shown refer to the BrS differential cross section $\omega\, {\rm d}\sigma/{\rm d}\omega$ integrated over the angles of the emitted photon and the scattered electron:

$$\omega \frac{{\rm d}\sigma}{{\rm d}\omega} = \frac{\omega^2}{c^3} \frac{p_2}{p_1} \int_{4\pi} \int_{4\pi} \frac{{\rm d}\Omega_{\mathbf{p}_2}\, {\rm d}\Omega_{\mathbf{k}}}{(2\pi)^4} \sum_{\lambda} |f|^2 \,, \tag{26}$$

where the sum is carried out over the photon polarizations. When computing the amplitude of the process we have used the non-relativistic distorted partial-wave approximation to describe the wavefunctions of the projectile. The radial parts of the wavefunctions were obtained by solving the Schrödinger equation with a frozen-core potential. The atomic wavefunctions were considered within the Hartree-Fock approximation. More details on the DPWA formalism and the corresponding algorithms can be found in Amusia and Korol (1992), Korol *et al* (1995, 1997).

In figures 1-3, where the data for 5 and 25 keV electrons (as indicated) are presented for Ar, Kr, Xe, we compare cross sections of the following four types.

(i) The ordinary BrS (the dashed lines) cross section, ${\rm d}\sigma_{\rm ord}$. This was obtained by using the amplitude (11) in (26).

(ii) The exact total BrS cross section, ${\rm d}\sigma_{\rm tot}$, (the solid lines) was computed by taking into account the ordinary, eq. (11), and the polarizational, eqs. (12-14), parts of the amplitude. The atomic electron – photon interaction was treated within the frame of the random phase approximation with exchange (Amusia 1990).

(iii) The total BrS in the 'stripping' approximation, ${\rm d}\sigma_{\rm s}$, (the dotted lines). To calculate this spectrum we used the first term on the right-hand side of (20) when constructing the amplitude.

(iv) The total BrS in the 'stripping' approximation which utilizes the amplitude (25), ${\rm d}\tilde{\sigma}_{\rm s}$.

In figure 4 the BrS spectra ${\rm d}\sigma_{\rm ord}$, ${\rm d}\sigma_{\rm s}$ and ${\rm d}\tilde{\sigma}_{\rm s}$ are plotted for an electron-Au collision for the incident energies 5-50 keV (as indicated).

To discuss these results we first note that it is clearly seen that the polarizational BrS plays an important role in the formation of the total BrS spectrum. Instead of smooth curves, typical for ${\rm d}\sigma_{\rm ord}$, the total BrS curves (the solid lines) exhibit complicated ω dependence characterized by powerful maxima and quite narrow cusps in the vicinity

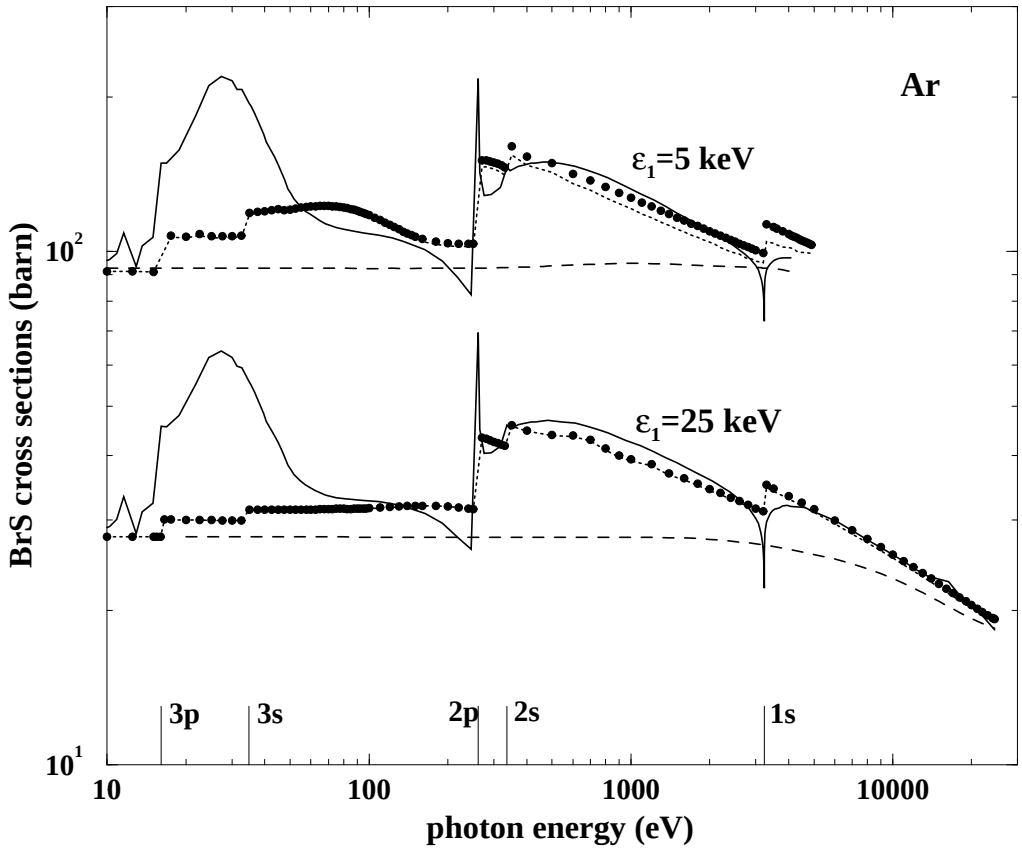

Figure 1. BrS spectra, $\omega\,\mathrm{d}\sigma/\mathrm{d}\omega$, formed in collision of $\varepsilon = 5$ keV and $\varepsilon = 25$ keV electrons with an Ar atom. The dashed curves describe the ordinary BrS, the dotted lines correspond to the 'stripping' approximation as outlined in section 2. The dots represent the cross sections obtained within the scheme described in section 3. The solid lines represent the total BrS spectra calculated within the distorted partial waves approximation without the use of the 'stripping' approximation. Vertical lines mark the Hartree-Fock ionization potentials of the atomic subshells. See also explanations in the text.

of the ionization thresholds. Such a behavior is totally due to the contribution of the polarizational, $\mathrm{d}\sigma_{\mathrm{pol}}$, as well as of the interference, $\mathrm{d}\sigma_{\mathrm{int}}$, terms to the total BrS spectrum. In the region $\omega < I_{1s}$ the wide maxima are mainly due to the virtual excitations of the atomic many-electron *nd*- and *np*-subshells. More detailed discussion of the behaviour and the peculiarities of the total BrS cross section over the wide range of the photon energies can be found in (Korol *et al* 1997).

The figures demonstrate that, apart from the region of comparatively low ω (which are $\omega < I_{2s} \approx 335$ eV for Ar, $\omega < I_{3s} \approx 295$ eV for Kr and $\omega < I_{4s} \approx 214$ eV for Xe),

the (exact) total curves are reproduced quite well if one considers the real part of the total BrS amplitude within the 'stripping' approximations. The noticeable deviations in the range of low ω values are not surprising. Indeed, the first maxima in the total BrS spectrum for Ar and Kr, and the first two maxima in the case of Xe, are due to the contribution of the real excitations of atomic electrons (see (14) and the second term in (20)). The amplitude $f_{\rm pol}^{\rm (i)}$, being used in (26), produces an additive term in the BrS cross section proportional to the photoabsorption cross section (Amusia *et al* 1975, Korol *et al* 1997). In our present calculations the quantity $f_{\rm pol}^{\rm (i)}$ was not taken into account when calculating the spectra in the 'stripping' approximation(s).

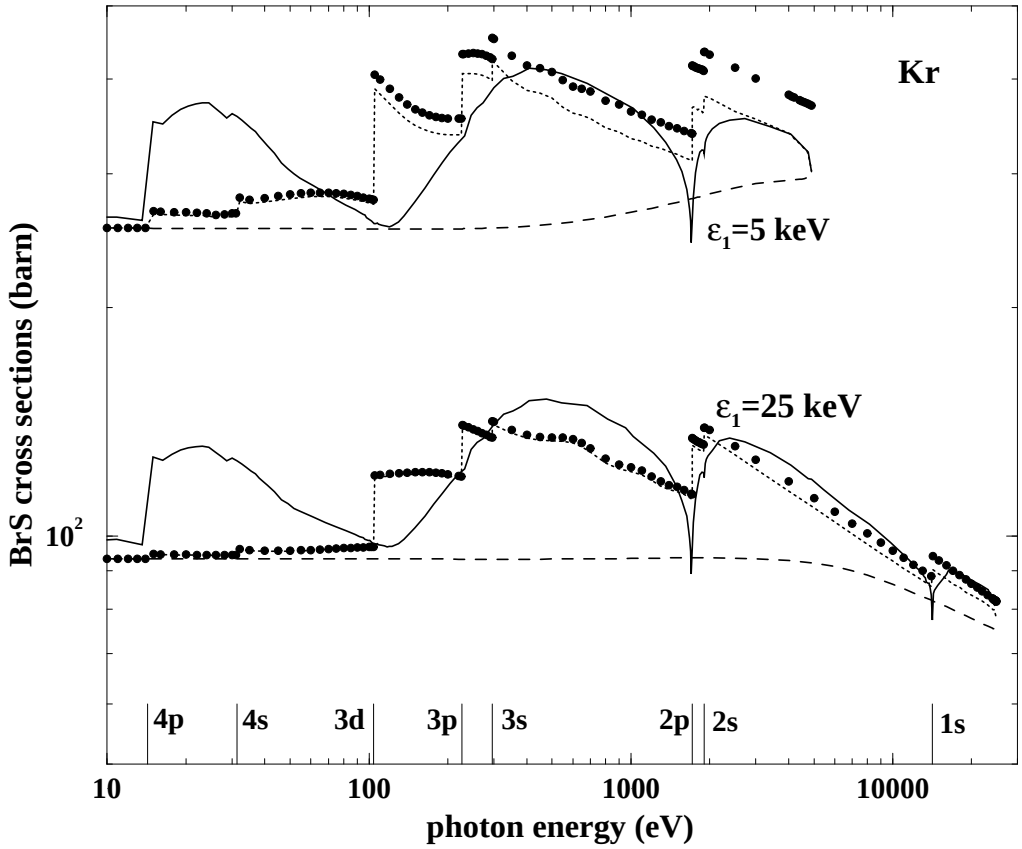

Figure 2. Same as in figure 1 but for a Kr atom.

Now let us turn to the comparison of the data obtained by means of the two different approaches to the 'stripping' approximation as discussed in sections 2 and 3. For this one compares the dotted lines and the dots in figures 1-3.

The general conclusion is that both approximate methods agree fairly well with each other. In the worst case, for the hard photon region of the Gold atom at low electron

energy, the difference between data obtained in the two approximations does not exceed 13%, but usually the differences are less than 10%.

We note that the agreement between the approaches is very good if the parameter $\nu = Z/p \leq 1$, where p is the momentum of the incident electron. It is worse if ν significantly exceeds unity. For a fixed target and for a given photon energy the discrepancy $\delta(Z, \varepsilon, \omega) = \mathrm{d}\tilde{\sigma}_\mathrm{s}/\mathrm{d}\sigma_\mathrm{s}$ increases with decrease of the incident energy ε. For a fixed incident energy $\delta(Z, \varepsilon, \omega)$ is an increasing function of Z.

As a function of photon energy the ratio $\delta(Z, \varepsilon, \omega)$ tends to unity on the left wing of the spectrum. This is evident since both matrix elements characterizing the 'stripping' amplitudes, the first term in (20) and the one given by (25), have the same limit as $\omega \longrightarrow 0$ (see the discussion at the end of section 3). The agreement becomes poorer as the fraction of radiated energy ω/ε increases.

Finally, it is interesting to note that in all cases the BrS cross sections results based on the approach of Avdonina and Pratt (1999) are bigger than those obtained using the approach of Korol *et al* (1999), i. e. their ratio $\delta(Z, \varepsilon, \omega) \geq 1$.

5. Concluding remarks

The main goal of this paper was to analyze the applicability of two different formulations of the 'stripping' approximation in the theory of bremsstrahlung process during non-relativistic electron-atom collisions. We have done this by presenting a detailed analysis of the formal arguments lying behind these theoretical schemes, and by performing numerical calculation of the BrS cross sections over a wide range of the dipole-photon energies, and for representative sets of atomic targets and non-relativistic electron energies. The numerical data obtained within the frameworks of both approaches were compared between themselves and with predictions of a more rigorous theory of BrS.

It has been demonstrated that both approximate methods, agreeing mostly very well with each other, reproduce also quite accurately the exact curves over a wide range of the photon energies, except for regions near the ionization thresholds I_j. In the regions $\omega \sim I_j$ the correspondence between the approximate and the exact curves can be improved by accounting for the imaginary part of the polarizational BrS amplitude (see (14)), which was omitted in the present consideration of the 'stripping' approximation.

The results of the calculations in the two 'stripping' approximations are very close to each other for most cases considered in this paper. The agreement is worse for small incident electron energies and for higher Z atoms, but even in the worst cases the results differ by not more than about 10%.

We would like to stress that the 'stripping' approximation represents by itself a very efficient method for calculating the characteristics of the BrS process (the spectral and spectral-angular distributions) in the whole range of photon energies. Indeed,

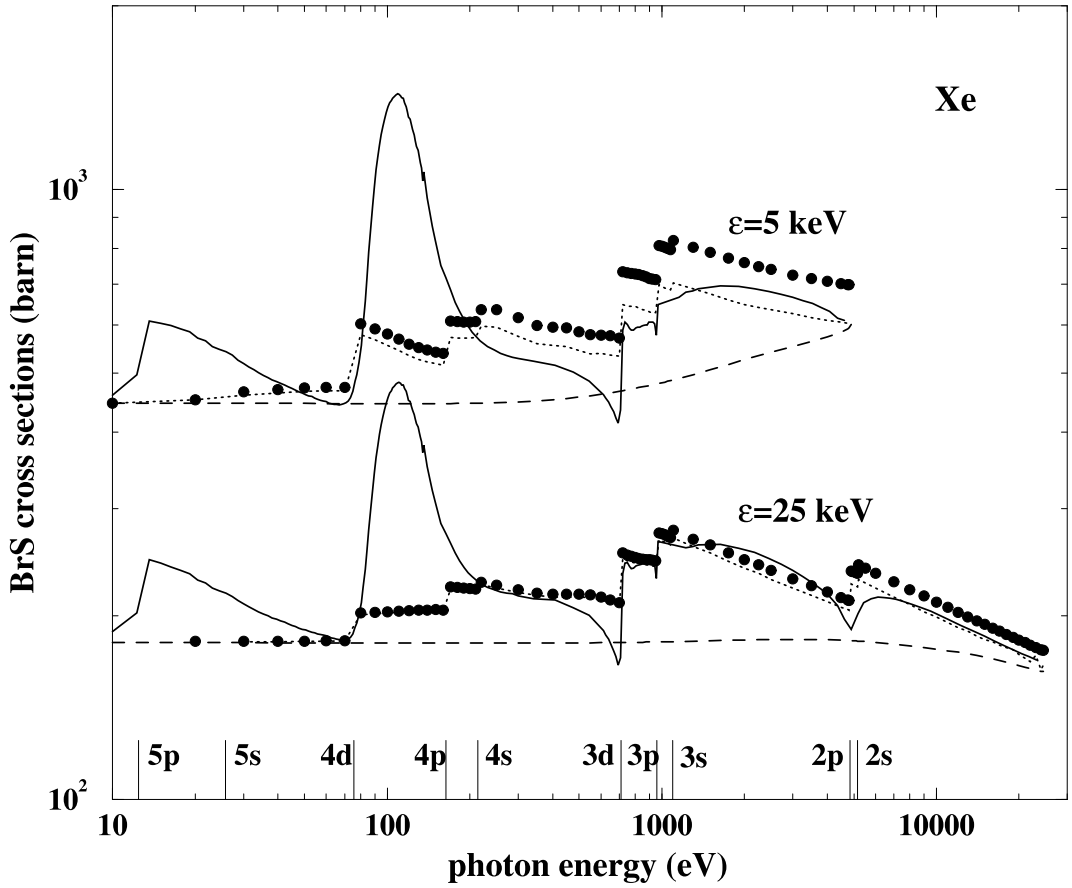

Figure 3. Same as in figure 1 but for a Xe atom.

this approach allows one to treat the total BrS amplitude as a single-electron free-free transition under the action of a local operator of the effective acceleration. This results in a considerable reduction of the computational efforts in comparison with those needed for the exact calculations (see, e.g., Korol and Solov'yov 1997).

The parametrization formula for the ordinary BrS spectra of neutral atoms and ions proposed recently by Avdonina and Pratt (1997a,b, 1999) allows to further simplify calculations of the total BrS spectra. The good agreement of two approaches compared in this paper gives us further justification of the applicability of these formula. Since the accuracy of the parametrization, comparing with the partial wave approach, is generally better then the accuracy of the 'stripping' approximation (see Avdonina and Pratt 1999 and the results of this paper), the analytical expressions should work very well for all atoms and for most of the bremsstrahlung spectrum, except for the spectrum near ionization thresholds, at least at the energies considered in this paper, $10\,keV \leq \varepsilon \leq 50\,keV$.

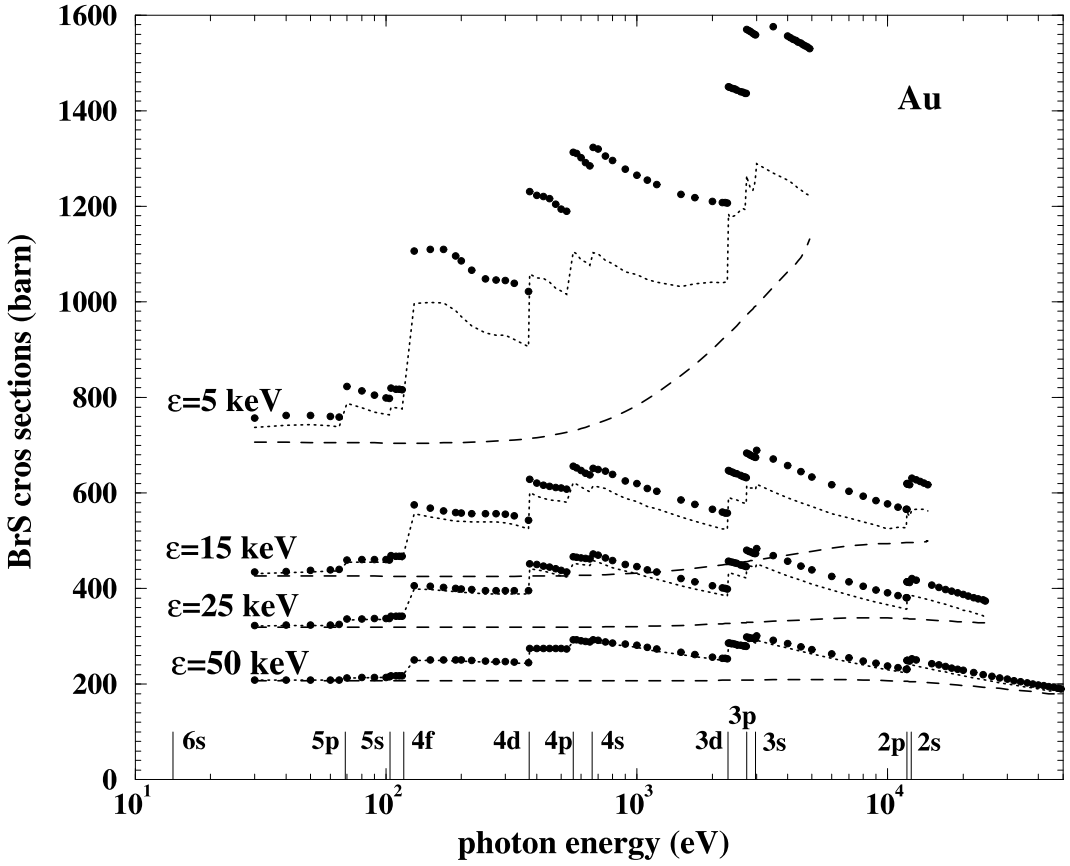

Figure 4. BrS spectra, $\omega\, \mathrm{d}\sigma/\mathrm{d}\omega$, formed in collision of electrons of various initial energies (as indicated) with an Au atom. The dashed curves describe the ordinary BrS, the solid lines correspond to the 'stripping' approximation as outlined in section 2. The dotted represent the cross sections obtained within the scheme described in section 3.

It is not clear how the approaches work for lower energies. One can see that at low energy the approach of Korol *et al* (1999) may be better in the hard photon region and/or for heavier atoms. Further investigation of the BrS spectrum at lower energies would be desirable.

In this paper we have restricted ourselves to the case of non-relativistic projectiles and dipole photons. Strictly speaking, the physics arguments leading to the 'stripping' effect are valid within these limits only. Nevertheless, it would be desirable to clarify in more detail whether the range of validity of the 'stripping' approximation (or its analogue) can be extended.

The paper of Avdonina and Pratt (1999) included an attempt to construct approximate expressions which simplify the complicated problem of obtaining total

BrS cross section from electrons of low relativistic energies. In Korol *et al* (2001) a generalization of the non-relativistic 'stripping' formula was derived for arbitrary energies of projectile, including relativistic ones, and taking into account the multipole character of the emission. A next logical step is to carry out a comprehensive comparison between the approaches of Avdonina and Pratt (1999) and Korol *et al* (2001).

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